

# Package ‘Compositional’

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**Title** Compositional Data Analysis

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**Depends** R (>= 4.0)

**Imports** bigstatsr, cluster, doParallel, emplik, energy, foreach,  
glmnet, graphics, grDevices, quantreg, MASS, Matrix, mda,  
minpack.lm, mixture, nnet, quadprog, Rfast, Rfast2, Rnanoflann,  
sn, stats

**Suggests** bigparallelr, codalm, FlexDir

**Description** Regression, classification, contour plots, hypothesis testing and fitting of distributions for compositional data are some of the functions included. We further include functions for percentages (or proportions).

The standard textbook for such data is John Aitchison's (1986) ``The statistical analysis of compositional data''. Relevant papers include:

a) Tsagris M.T., Preston S. and Wood A.T.A. (2011). ``A data-based power transformation for compositional data''. Fourth International International Workshop on Compositional Data Analysis. <doi:10.48550/arXiv.1106.1451>

b) Tsagris M. (2014). ``The k-NN algorithm for compositional data: a revised approach with and without zero values present''. Journal of Data Science, 12(3): 519--534. <doi:10.6339/JDS.201407\_12(3).0008>.

c) Tsagris M. (2015). ``A novel, divergence based, regression for compositional data''. Proceedings of the 28th Panhellenic Statistics Conference, 15-18 April 2015, Athens, Greece, 430--444. <doi:10.48550/arXiv.1511.07600>.

d) Tsagris M. (2015). ``Regression analysis with compositional data containing zero values''. Chilean Journal of Statistics, 6(2): 47--57. <[https://soche.cl/chjs/volumes/06/02/Tsagris\(2015\).pdf](https://soche.cl/chjs/volumes/06/02/Tsagris(2015).pdf)>.

- e) Tsagris M., Preston S. and Wood A.T.A. (2016). "Improved supervised classification for compositional data using the alpha-transformation". *Journal of Classification*, 33(2): 243--261. <doi:10.1007/s00357-016-9207-5>.
- f) Tsagris M., Preston S. and Wood A.T.A. (2017). "Nonparametric hypothesis testing for equality of means on the simplex". *Journal of Statistical Computation and Simulation*, 87(2): 406--422. <doi:10.1080/00949655.2016.1216554>.
- g) Tsagris M. and Stewart C. (2018). "A Dirichlet regression model for compositional data with zeros". *Lobachevskii Journal of Mathematics*, 39(3): 398--412. <doi:10.1134/S1995080218030198>.
- h) Alenazi A. (2019). "Regression for compositional data with compositional data as predictor variables with or without zero values". *Journal of Data Science*, 17(1): 219--238. <doi:10.6339/JDS.201901\_17(1).0010>.
- i) Tsagris M. and Stewart C. (2020). "A folded model for compositional data analysis". *Australian and New Zealand Journal of Statistics*, 62(2): 249--277. <doi:10.1111/anzs.12289>.
- j) Alenazi A.A. (2022). "f-divergence regression models for compositional data". *Pakistan Journal of Statistics and Operation Research*, 18(4): 867--882. <doi:10.18187/pjsor.v18i4.3969>.
- k) Tsagris M. and Stewart C. (2022). "A Review of Flexible Transformations for Modeling Compositional Data". In *Advances and Innovations in Statistics and Data Science*, pp. 225--234. <doi:10.1007/978-3-031-08329-7\_10>.
- l) Alenazi A. (2023). "A review of compositional data analysis and recent advances". *Communications in Statistics--Theory and Methods*, 52(16): 5535--5567. <doi:10.1080/03610926.2021.2014890>.
- m) Tsagris M., Alenazi A. and Stewart C. (2023). "Flexible non-parametric regression models for compositional response data with zeros". *Statistics and Computing*, 33(106). <doi:10.1007/s11222-023-10277-5>.
- n) Tsagris. M. (2024). "Constrained least squares simplicial-simplicial regression". <doi:10.48550/arXiv.2403.19835>.

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## Contents

Compositional-package . . . . .	7
Aitchison's test for two mean vectors and/or covariance matrices . . . . .	8
All pairwise additive log-ratio transformations . . . . .	9
Alpha-generalised correlations between two compositional datasets . . . . .	10
ANOVA for the log-contrast GLM versus the unconstrained GLM . . . . .	12
ANOVA for the log-contrast regression versus the unconstrained linear regression . . . . .	13
Beta regression . . . . .	14
Column-wise MLE of some univariate distributions . . . . .	15
Contour plot of mixtures of Dirichlet distributions in $S^2$ . . . . .	16
Contour plot of the alpha multivariate normal in $S^2$ . . . . .	17

Contour plot of the alpha-folded model in $S^2$ . . . . .	18
Contour plot of the Dirichlet distribution in $S^2$ . . . . .	20
Contour plot of the Flexible Dirichlet distribution in $S^2$ . . . . .	21
Contour plot of the Gaussian mixture model in $S^2$ . . . . .	22
Contour plot of the generalised Dirichlet distribution in $S^2$ . . . . .	23
Contour plot of the kernel density estimate in $S^2$ . . . . .	24
Contour plot of the normal distribution in $S^2$ . . . . .	26
Contour plot of the skew skew-normal distribution in $S^2$ . . . . .	27
Contour plot of the t distribution in $S^2$ . . . . .	28
Cross validation for some compositional regression models . . . . .	29
Cross validation for the alpha-k-NN regression with compositional predictor variables . . . . .	30
Cross validation for the alpha-k-NN regression with compositional response data . . . . .	32
Cross validation for the alpha-kernel regression with compositional response data . . . . .	33
Cross validation for the kernel regression with Euclidean response data . . . . .	35
Cross validation for the regularised and flexible discriminant analysis with compositional data using the alpha-transformation . . . . .	36
Cross validation for the ridge regression . . . . .	38
Cross validation for the ridge regression with compositional data as predictor using the alpha-transformation . . . . .	40
Cross validation for the TFLR model . . . . .	42
Cross-validation for LASSO with compositional predictors using the alpha-transformation . . . . .	43
Cross-validation for the alpha-SCLS model . . . . .	45
Cross-validation for the alpha-TFLR model . . . . .	46
Cross-validation for the Dirichlet discriminant analysis . . . . .	47
Cross-validation for the LASSO Kullback-Leibler divergence based regression . . . . .	48
Cross-validation for the LASSO log-ratio regression with compositional response . . . . .	50
Cross-validation for the naive Bayes classifiers for compositional data . . . . .	51
Cross-validation for the naive Bayes classifiers for compositional data using the alpha-transformation . . . . .	52
Cross-validation for the SCLS model . . . . .	54
Cross-validation for the SCRQ model . . . . .	55
Density of compositional data from Gaussian mixture models . . . . .	56
Density of the Flexible Dirichlet distribution . . . . .	58
Density of the folded normal distribution . . . . .	59
Density values of a Dirichlet distribution . . . . .	60
Density values of a generalised Dirichlet distribution . . . . .	61
Density values of a mixture of Dirichlet distributions . . . . .	62
Dirichlet discriminant analysis . . . . .	63
Dirichlet random values simulation . . . . .	64
Dirichlet regression . . . . .	65
Distance based regression models for proportions . . . . .	67
Divergence based regression for compositional data . . . . .	69
Divergence based regression for compositional data with compositional data in the co-variates side using the alpha-transformation . . . . .	71
Divergence matrix of compositional data . . . . .	73
Empirical likelihood hypothesis testing for two mean vectors . . . . .	74
Energy test of equality of distributions using the alpha-transformation . . . . .	76
Estimating location and scatter parameters for compositional data . . . . .	77

Estimation of the probability left outside the simplex when using the alpha-transformation	78
Estimation of the value of alpha in the folded model	80
Estimation of the value of alpha via the profile log-likelihood	81
Exponential empirical likelihood hypothesis testing for two mean vectors	82
Fast estimation of the value of alpha	85
Gaussian mixture models for compositional data	86
Gaussian mixture models for compositional data using the alpha-transformation	88
Generalised Dirichlet random values simulation	90
Generate random folds for cross-validation	91
Greenacre's power transformation	92
Helper Frechet mean for compositional data	93
Helper functions for the Kullback-Leibler regression	94
Hotelling's multivariate version of the 2 sample t-test for Euclidean data	96
Hypothesis testing for two or more compositional mean vectors	98
ICE plot for projection pursuit regression with compositional predictor variables	99
ICE plot for the alpha-k-NN regression	101
ICE plot for the alpha-kernel regression	102
ICE plot for univariate kernel regression	103
Inverse of the alpha-transformation	105
James multivariate version of the t-test	106
Kernel regression with a numerical response vector or matrix	108
Kullback-Leibler divergence and Bhattacharyya distance between two Dirichlet distributions	109
LASSO Kullback-Leibler divergence based regression	110
LASSO log-ratio regression with compositional response	112
LASSO with compositional predictors using the alpha-transformation	113
Log-contrast GLMs with compositional predictor variables	115
Log-contrast logistic or Poisson regression with with multiple compositional predictors	116
Log-contrast quantile regression with compositional predictor variables	118
Log-contrast quantile regression with with multiple compositional predictors	119
Log-contrast regression with compositional predictor variables	121
Log-contrast regression with multiple compositional predictors	122
Log-likelihood ratio test for a Dirichlet mean vector	124
Log-likelihood ratio test for a symmetric Dirichlet distribution	125
Minimized Kullback-Leibler divergence between Dirichlet and logistic normal	126
Mixture model selection via BIC	127
Mixture model selection with the alpha-transformation using BIC	128
MLE for the multivariate t distribution	130
MLE of distributions defined in the (0, 1) interval	131
MLE of the Dirichlet distribution	133
MLE of the Dirichlet distribution via Newton-Raphson	134
MLE of the folded model for a given value of alpha	135
MLE of the zero adjusted Dirichlet distribution	137
Multivariate analysis of variance (James test)	138
Multivariate analysis of variance assuming equality of the covariance matrices	139
Multivariate kernel density estimation	140
Multivariate kernel density estimation for compositional data	142
Multivariate linear regression	143

Multivariate normal random values simulation on the simplex . . . . .	144
Multivariate or univariate regression with compositional data in the covariates side using the alpha-transformation . . . . .	145
Multivariate regression with compositional data . . . . .	147
Multivariate skew normal random values simulation on the simplex . . . . .	148
Multivariate t random values simulation on the simplex . . . . .	150
Naive Bayes classifiers for compositional data . . . . .	151
Naive Bayes classifiers for compositional data using the alpha-transformation . . . . .	152
Non linear least squares regression for compositional data . . . . .	154
Non-parametric zero replacement strategies . . . . .	155
Permutation linear independence test in the SCLS model . . . . .	156
Permutation linear independence test in the TFLR model . . . . .	157
Permutation test for the matrix of coefficients in the SCLS model . . . . .	158
Permutation test for the matrix of coefficients in the TFLR model . . . . .	160
Perturbation operation . . . . .	161
Plot of the LASSO coefficients . . . . .	162
Power operation . . . . .	163
Principal component analysis . . . . .	164
Principal component analysis using the alpha-transformation . . . . .	165
Principal component generalised linear models . . . . .	166
Principal coordinate analysis using the alpha-distance . . . . .	168
Principal coordinate analysis using the Jensen-Shannon divergence . . . . .	169
Projection pursuit regression for compositional data . . . . .	170
Projection pursuit regression with compositional predictor variables . . . . .	171
Projection pursuit regression with compositional predictor variables using the alpha- transformation . . . . .	172
Projections based test for distributional equality of two groups . . . . .	174
Proportionality correlation coefficient matrix . . . . .	175
Quasi binomial regression for proportions . . . . .	176
Random values generation from some univariate distributions defined on the (0,1) interval	177
Read a file as a Filebacked Big Matrix . . . . .	178
Regression with compositional data using the alpha-transformation . . . . .	179
Regularised and flexible discriminant analysis for compositional data using the alpha- transformation . . . . .	181
Regularised discriminant analysis for Euclidean data . . . . .	183
Ridge regression . . . . .	184
Ridge regression plot . . . . .	185
Ridge regression with compositional data in the covariates side using the alpha-transformation	187
Ridge regression with the alpha-transformation plot . . . . .	188
Simplicial constrained median regression for compositional responses and predictors model . . . . .	189
Simulation of compositional data from Gaussian mixture models . . . . .	191
Simulation of compositional data from mixtures of Dirichlet distributions . . . . .	192
Simulation of compositional data from the Flexible Dirichlet distribution . . . . .	193
Simulation of compositional data from the folded normal distribution . . . . .	194
Spatial median regression . . . . .	195
Ternary diagram . . . . .	196
Ternary diagram of regression models . . . . .	198

Ternary diagram with confidence region for the matrix of coefficients of the SCLS or the TFLR model . . . . .	199
Ternary diagram with confidence region for the mean . . . . .	200
Ternary diagram with the coefficients of the simplicial-simplicial regression models . . .	201
The additive log-ratio transformation and its inverse . . . . .	202
The alpha-distance . . . . .	203
The alpha-IT transformation . . . . .	205
The alpha-IT-distance . . . . .	206
The alpha-k-NN regression for compositional response data . . . . .	207
The alpha-k-NN regression with compositional predictor variables . . . . .	208
The alpha-kernel regression with compositional response data . . . . .	210
The alpha-SCLS model . . . . .	211
The alpha-TFLR model . . . . .	212
The alpha-transformation . . . . .	213
The Box-Cox transformation applied to ratios of components . . . . .	215
The ESOV-distance . . . . .	216
The folded power transformation . . . . .	217
The Frechet mean for compositional data . . . . .	218
The Helmert sub-matrix . . . . .	219
The k-nearest neighbours using the alpha-distance . . . . .	220
The k-NN algorithm for compositional data . . . . .	222
The multiplicative log-ratio transformation and its inverse . . . . .	224
The pivot coordinate transformation and its inverse . . . . .	225
The SCLS model . . . . .	226
The SCLS model with multiple compositional predictors . . . . .	227
The TFLR model with multiple compositional predictors . . . . .	228
The transformation-free linear regression (TFLR) for compositional responses and predictors . . . . .	230
Total variability . . . . .	231
Tuning of the alpha-generalised correlations between two compositional datasets . . . .	232
Tuning of the bandwidth $h$ of the kernel using the maximum likelihood cross validation .	233
Tuning of the divergence based regression for compositional data with compositional data in the covariates side using the alpha-transformation . . . . .	235
Tuning of the k-NN algorithm for compositional data . . . . .	236
Tuning of the projection pursuit regression for compositional data . . . . .	239
Tuning of the projection pursuit regression with compositional predictor variables . . . .	240
Tuning of the projection pursuit regression with compositional predictor variables using the alpha-transformation . . . . .	241
Tuning the number of PCs in the PCR with compositional data using the alpha-transformation	243
Tuning the parameters of the regularised discriminant analysis . . . . .	245
Tuning the principal components with GLMs . . . . .	246
Tuning the value of alpha in the alpha-regression . . . . .	248
Two-sample test of high-dimensional means for compositional data . . . . .	250
Unconstrained GLMs with compositional predictor variables . . . . .	251
Unconstrained linear regression with compositional predictor variables . . . . .	252
Unconstrained linear regression with multiple compositional predictors . . . . .	254
Unconstrained logistic or Poisson regression with multiple compositional predictors . . .	255
Unconstrained quantile regression with compositional predictor variables . . . . .	257

Unconstrained quantile regression with multiple compositional predictors . . . . .	258
Unit-Weibull regression models for proportions . . . . .	260
Zero adjusted Dirichlet regression . . . . .	261

<b>Index</b>	<b>263</b>
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Compositional-package *Compositional Data Analysis*

---

## Description

A Collection of Functions for Compositional Data Analysis.

## Details

Package: Compositional  
Type: Package  
Version: 7.2  
Date: 2024-12-04  
License: GPL-2

## Maintainers

Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>

## Note

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Ermanno Affuso from the university of South Alabama suggested that I have a default value in the function `mkde`.

Van Thang Hoang from Hasselt university spotted a bug in the function `js.compreg`.

Claudia Wehrhahn Cortes spotted a bug in the function `diri.reg`.

Philipp Kynast from Bruker Daltonik GmbH found a mistake in the function `mkde` which is now fixed.

Jasmine Heyse from the university of Ghent spotted a bug in the function `kl.compreg` which is now fixed.

Magne Neby suggested to add names in the covariance matrix of the divergence based regression models.

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Charlotte Fabri and Laura Byrne spotted a possible problem in the function `zadr`.

Levi Bankston found a bug in the bootstrap version of the function `kl.compreg`.

Sucharitha Dodamgodage suggested to add an extra case in the function `dirimean.test`.

Loic Mangnier found a bug in the function `lc.glm` which is now fixed and also became faster.

Ravi Varadhan found a bug in `diri.reg` and he is acknowledged for that.

### Author(s)

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### References

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

---

Aitchison's test for two mean vectors and/or covariance matrices

*Aitchison's test for two mean vectors and/or covariance matrices*

---

### Description

Aitchison's test for two mean vectors and/or covariance matrices.

### Usage

```
ait.test(x1, x2, type = 1, alpha = 0.05)
```

### Arguments

<code>x1</code>	A matrix containing the compositional data of the first sample. Zeros are not allowed.
<code>x2</code>	A matrix containing the compositional data of the second sample. Zeros are not allowed.
<code>type</code>	The type of hypothesis test to perform. Type=1 refers to testing the equality of the mean vectors and the covariance matrices. Type=2 refers to testing the equality of the covariance matrices. Type=2 refers to testing the equality of the mean vectors.
<code>alpha</code>	The significance level, set to 0.05 by default.



**Details**

The test is described in Aitchison (2003). See the references for more information.

**Value**

A vector with the test statistic, the p-value, the critical value and the degrees of freedom of the chi-square distribution.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

John Aitchison (2003). The Statistical Analysis of Compositional Data, p. 153-157. Blackburn Press.

**See Also**

[comp.test](#)

**Examples**

```
x1 <- as.matrix(iris[1:50, 1:4])
x1 <- x1 / rowSums(x1)
x2 <- as.matrix(iris[51:100, 1:4])
x2 <- x2 / rowSums(x2)
ait.test(x1, x2, type = 1)
ait.test(x1, x2, type = 2)
ait.test(x1, x2, type = 3)
```

---

All pairwise additive log-ratio transformations

*All pairwise additive log-ratio transformations*

---

**Description**

All pairwise additive log-ratio transformations.

**Usage**

```
alr.all(x)
```

**Arguments**

x                    A numerical matrix with the compositional data.

**Details**

The additive log-ratio transformation with the first component being the common divisor is applied. Then all the other pairwise log-ratios are computed and added next to each column. For example, divide by the first component, then divide by the second component and so on. This means that no zeros are allowed.

**Value**

A matrix with all pairwise alr transformed data.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

**See Also**

[alr](#), [alfa](#)

**Examples**

```
x <- as.matrix(iris[, 2:4])
x <- x / rowSums(x)
y <- alr.all(x)
```

---

Alpha-generalised correlations between two compositional datasets  
 *$\alpha$ -generalised correlations between two compositional datasets*

---

**Description**

$\alpha$ -generalised correlations between two compositional datasets.

**Usage**

```
acor(y, x, a, type = "dcor")
```

**Arguments**

y	A matrix with the compositional data.
x	A matrix with the compositional data.
a	The value of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ the isometric log-ratio transformation is applied. If more than one values are supplied the distance or canonical correlation are computed for all values.
type	The type of correlation to compute, the distance correlation ("edist"), the canonical correlation ("cancor") or "both".

**Details**

The  $\alpha$ -transformation is applied to each composition and then the distance correlation or the canonical correlation is computed. If one value of  $\alpha$  is supplied the type="cancor" will return all eigenvalues. If more than one values of  $\alpha$  are provided then the first eigenvalue only will be returned.

**Value**

A vector or a matrix depending on the length of the values of  $\alpha$  and the type of the correlation to be computed.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

G.J. Szekely, M.L. Rizzo and N. K. Bakirov (2007). Measuring and Testing Independence by Correlation of Distances. *Annals of Statistics*, 35(6): 2769-2794.

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In *Proceedings of the 4th Compositional Data Analysis Workshop*, Girona, Spain. <https://arxiv.org/pdf/1106.1451.pdf>

**See Also**

[acor.tune](#), [aeqdist.etest](#), [alfa](#), [alfa.profile](#)

**Examples**

```
y <- rdiri(30, runif(3) )
x <- rdiri(30, runif(4) )
acor(y, x, a = 0.4)
```

---

ANOVA for the log-contrast GLM versus the unconstrained GLM

*ANOVA for the log-contrast GLM versus the unconstrained GLM*

---

## Description

ANOVA for the log-contrast GLM versus the unconstrained GLM.

## Usage

```
lcfglm.aov(mod0, mod1)
```

## Arguments

mod0	The log-contrast GLM. The object returned by <code>lc.glm</code> .
mod1	The unconstrained GLM. The object returned by <code>ulc.glm</code> .

## Details

A chi-square test is performed to test the zero-to-sum constraints of the regression coefficients.

## Value

A vector with two values, the chi-square test statistic and its associated p-value.

## Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

## See Also

[lc.glm](#), [ulc.glm](#)

## Examples

```
y <- rbinom(150, 1, 0.5)
x <- as.matrix(iris[, 2:4])
x <- x / rowSums(x)
mod0 <- lc.glm(y, x)
mod1 <- ulc.glm(y, x)
lcfglm.aov(mod0, mod1)
```

---

ANOVA for the log-contrast regression versus the unconstrained linear regression

*ANOVA for the log-contrast regression versus the unconstrained linear regression*

---

### Description

ANOVA for the log-contrast regression versus the unconstrained linear regression.

### Usage

```
lcreg.aov(mod0, mod1)
```

### Arguments

`mod0`            The log-contrast regression model. The object returned by [lc.reg](#).  
`mod1`            The unconstrained linear regression model. The object returned by [ulc.reg](#).

### Details

An F-test is performed to test the zero-to-sum constraints of the regression coefficients.

### Value

A vector with two values, the F test statistic and its associated p-value.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

### See Also

[lc.reg](#), [ulc.reg](#), [alfa.pcr](#), [alfa.knn.reg](#)

### Examples

```
y <- iris[, 1]
x <- as.matrix(iris[, 2:4])
x <- x / rowSums(x)
mod0 <- lc.reg(y, x)
mod1 <- ulc.reg(y, x)
lcreg.aov(mod0, mod1)
```

---

Beta regression      *Beta regression*

---

**Description**

Beta regression.

**Usage**

```
beta.reg(y, x, xnew = NULL)
```

**Arguments**

y	The response variable. It must be a numerical vector with proportions excluding 0 and 1.
x	The independent variable(s). It can be a vector, a matrix or a dataframe with continuous only variables, a data frame with mixed or only categorical variables.
xnew	If you have new values for the predictor variables (dataset) whose response values you want to predict insert them here.

**Details**

Beta regression is fitted.

**Value**

A list including:

phi	The estimated precision parameter.
info	A matrix with the estimated regression parameters, their standard errors, Wald statistics and associated p-values.
loglik	The log-likelihood of the regression model.
est	The estimated values if xnew is not NULL.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Ferrari S.L.P. and Cribari-Neto F. (2004). Beta Regression for Modelling Rates and Proportions. Journal of Applied Statistics, 31(7): 799-815.

**See Also**

[beta.est](#), [propreg](#), [diri.reg](#)

**Examples**

```
y <- rbeta(300, 3, 5)
x <- matrix( rnorm(300 * 2), ncol = 2)
beta.reg(y, x)
```

---

Column-wise MLE of some univariate distributions

*Column-wise MLE of some univariate distributions*

---

**Description**

Column-wise MLE of some univariate distributions.

**Usage**

```
colbeta.est(x, tol = 1e-07, maxiters = 100, parallel = FALSE)
collogitnorm.est(x)
colunitweibull.est(x, tol = 1e-07, maxiters = 100, parallel = FALSE)
colzillogitnorm.est(x)
```

**Arguments**

x	A numerical matrix with data. Each column refers to a different vector of observations of the same distribution. The values must be percentages, excluding 0 and 1,
tol	The tolerance value to terminate the Newton-Fisher algorithm.
maxiters	The maximum number of iterations to implement.
parallel	Do you want to calculations to take place in parallel? The default value is FALSE

**Details**

For each column, the same distribution is fitted and its parameters and log-likelihood are computed.

**Value**

A matrix with two, three or four columns. The first one, two or three columns contain the parameter(s) of the distribution, while the last column contains the relevant log-likelihood.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

- N.L. Johnson, S. Kotz & N. Balakrishnan (1994). Continuous Univariate Distributions, Volume 1 (2nd Edition).
- N.L. Johnson, S. Kotz & N. Balakrishnan (1970). Distributions in statistics: continuous univariate distributions, Volume 2.
- J. Mazucheli, A. F. B. Menezes, L. B. Fernandes, R. P. de Oliveira & M. E. Ghitany (2020). The unit-Weibull distribution as an alternative to the Kumaraswamy distribution for the modeling of quantiles conditional on covariates. Journal of Applied Statistics, DOI:10.1080/02664763.2019.1657813.

**See Also**

[beta.est](#)

**Examples**

```
x <- matrix( rbeta(200, 3, 4), ncol = 4 )
a <- colbeta.est(x)
```

---

Contour plot of mixtures of Dirichlet distributions in  $S^2$   
*Contour plot of mixtures of Dirichlet distributions in  $S^2$*

---

**Description**

Contour plot of mixtures of Dirichlet distributions in  $S^2$ .

**Usage**

```
mixdiri.contour(a, prob, n = 100, x = NULL, cont.line = FALSE)
```

**Arguments**

a	A matrix where each row contains the parameters of each Dirichlet distribution.
prob	A vector with the mixing probabilities.
n	The number of grid points to consider over which the density is calculated.
x	This is either NULL (no data) or contains a 3 column matrix with compositional data.
cont.line	Do you want the contour lines to appear? If yes, set this TRUE.

**Details**

The user can plot only the contour lines of a Dirichlet with a given vector of parameters, or can also add the relevant data should he/she wish to.



**Value**

A ternary diagram with the points and the Dirichlet contour lines.

**Author(s)**

Michail Tsagris and Christos Adam.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Christos Adam <pada4m4@gmail.com>.

**References**

Ng Kai Wang, Guo-Liang Tian and Man-Lai Tang (2011). Dirichlet and related distributions: Theory, methods and applications. John Wiley & Sons.

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

**See Also**

[diri.contour](#), [gendiri.contour](#), [compnorm.contour](#), [comp.kerncontour](#), [mix.compnorm.contour](#), [diri.nr](#), [dda](#)

**Examples**

```
a <- matrix( c(12, 30, 45, 32, 50, 16), byrow = TRUE, ncol = 3)
prob <- c(0.5, 0.5)
mixdiri.contour(a, prob)
```

---

Contour plot of the alpha multivariate normal in  $S^2$   
*Contour plot of the  $\alpha$  multivariate normal in  $S^2$*

---

**Description**

Contour plot of the  $\alpha$  multivariate normal in  $S^2$ .

**Usage**

```
alfa.contour(m, s, a, n = 100, x = NULL, cont.line = FALSE)
```

**Arguments**

m	The mean vector of the $\alpha$ multivariate normal model.
s	The covariance matrix of the $\alpha$ multivariate normal model.
a	The value of a for the $\alpha$ -transformation.
n	The number of grid points to consider over which the density is calculated.
x	This is either NULL (no data) or contains a 3 column matrix with compositional data.
cont.line	Do you want the contour lines to appear? If yes, set this TRUE.

**Details**

The  $\alpha$ -transformation is applied to the compositional data and then for a grid of points within the 2-dimensional simplex, the density of the  $\alpha$  multivariate normal is calculated and the contours are plotted.

**Value**

The contour plot of the  $\alpha$  multivariate normal appears.

**Author(s)**

Michail Tsagris and Christos Adam.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Christos Adam <pada4m4@gmail.com>.

**References**

Tsagris M. and Stewart C. (2022). A Review of Flexible Transformations for Modeling Compositional Data. In *Advances and Innovations in Statistics and Data Science*, pp. 225–234. [https://link.springer.com/chapter/10.1007/978-3-031-08329-7\\_10](https://link.springer.com/chapter/10.1007/978-3-031-08329-7_10)

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In *Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain*. <https://arxiv.org/pdf/1106.1451.pdf>

**See Also**

[folded.contour](#), [compnorm.contour](#), [diri.contour](#), [mix.compnorm.contour](#), [bivt.contour](#), [skewnorm.contour](#)

**Examples**

```
x <- as.matrix(iris[, 1:3])
x <- x / rowSums(x)
a <- a.est(x)$best
m <- colMeans(alfa(x, a)$aff)
s <- cov(alfa(x, a)$aff)
alfa.contour(m, s, a)
```

---

Contour plot of the alpha-folded model in  $S^2$

*Contour plot of the  $\alpha$ -folded model in  $S^2$*

---

**Description**

Contour plot of the  $\alpha$ -folded model in  $S^2$ .

**Usage**

```
folded.contour(mu, su, p, a, n = 100, x = NULL, cont.line = FALSE)
```

**Arguments**

mu	The mean vector of the folded model.
su	The covariance matrix of the folded model.
p	The probability inside the simplex of the folded model.
a	The value of $a$ for the $\alpha$ -transformation.
n	The number of grid points to consider over which the density is calculated.
x	This is either NULL (no data) or contains a 3 column matrix with compositional data.
cont.line	Do you want the contour lines to appear? If yes, set this TRUE.

**Details**

The  $\alpha$ -transformation is applied to the compositional data and then for a grid of points within the 2-dimensional simplex the folded model's density is calculated and the contours are plotted.

**Value**

The contour plot of the folded model appears.

**Author(s)**

Michail Tsagris and Christos Adam.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Christos Adam <pada4m4@gmail.com>.

**References**

Tsagris M. and Stewart C. (2022). A Review of Flexible Transformations for Modeling Compositional Data. In *Advances and Innovations in Statistics and Data Science*, pp. 225–234. [https://link.springer.com/chapter/10.1007/978-3-031-08329-7\\_10](https://link.springer.com/chapter/10.1007/978-3-031-08329-7_10)

Tsagris M. and Stewart C. (2020). A folded model for compositional data analysis. *Australian and New Zealand Journal of Statistics*, 62(2): 249-277. <https://arxiv.org/pdf/1802.07330.pdf>

**See Also**

[alfa.contour](#), [compnorm.contour](#), [diri.contour](#), [mix.compnorm.contour](#), [bivt.contour](#), [skewnorm.contour](#)

**Examples**

```
x <- as.matrix(iris[, 1:3])
x <- x / rowSums(x)
a <- a.est(x)$best
mod <- alpha.mle(x, a)
folded.contour(mod$mu, mod$su, mod$p, a)
```

---

Contour plot of the Dirichlet distribution in  $S^2$   
*Contour plot of the Dirichlet distribution in  $S^2$*

---

**Description**

Contour plot of the Dirichlet distribution in  $S^2$ .

**Usage**

```
diri.contour(a, n = 100, x = NULL, cont.line = FALSE)
```

**Arguments**

<code>a</code>	A vector with three elements corresponding to the 3 (estimated) parameters.
<code>n</code>	The number of grid points to consider over which the density is calculated.
<code>x</code>	This is either NULL (no data) or contains a 3 column matrix with compositional data.
<code>cont.line</code>	Do you want the contour lines to appear? If yes, set this TRUE.

**Details**

The user can plot only the contour lines of a Dirichlet with a given vector of parameters, or can also add the relevant data should he/she wish to.

**Value**

A ternary diagram with the points and the Dirichlet contour lines.

**Author(s)**

Michail Tsagris and Christos Adam.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Christos Adam <pada4m4@gmail.com>.

**References**

Ng Kai Wang, Guo-Liang Tian and Man-Lai Tang (2011). Dirichlet and related distributions: Theory, methods and applications. John Wiley & Sons.

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

**See Also**

[mixdiri.contour](#), [gendiri.contour](#), [compnorm.contour](#), [comp.kerncontour](#), [mix.compnorm.contour](#)

**Examples**

```
x <- as.matrix( iris[, 1:3] )
x <- x / rowSums(x)
diri.contour( a = c(3, 4, 2) )
```

---

Contour plot of the Flexible Dirichlet distribution in  $S^2$

*Contour plot of the Flexible Dirichlet distribution in  $S^2$*

---

**Description**

Contour plot of the Flexible Dirichlet distribution in  $S^2$ .

**Usage**

```
fd.contour(alpha, prob, tau, n = 100, x = NULL, cont.line = FALSE)
```

**Arguments**

alpha	A vector of the non-negative $\alpha$ parameters.
prob	A vector of the clusters' probabilities. It must sum to one.
tau	The non-negative scalar $\tau$ parameter.
n	The number of grid points to consider over which the density is calculated.
x	This is either NULL (no data) or contains a 3 column matrix with compositional data.
cont.line	Do you want the contour lines to appear? If yes, set this TRUE.

**Details**

The user can plot only the contour lines of a Dirichlet with a given vector of parameters, or can also add the relevant data should they wish to.

**Value**

A ternary diagram with the points and the Flexible Dirichlet contour lines.

**Author(s)**

Michail Tsagris and Christos Adam.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Christos Adam <pada4m4@gmail.com>.

**References**

Ongaro A. and Migliorati S. (2013). A generalization of the Dirichlet distribution. *Journal of Multivariate Analysis*, 114, 412–426.

Migliorati S., Ongaro A. and Monti G. S. (2017). A structured Dirichlet mixture model for compositional data: inferential and applicative issues. *Statistics and Computing*, 27, 963–983.

**See Also**

[compnorm.contour](#), [folded.contour](#), [bivt.contour](#), [comp.kerncontour](#), [mix.compnorm.contour](#)

**Examples**

```
fd.contour(alpha = c(10, 11, 12), prob = c(0.25, 0.25, 0.5), tau = 4)
```

---

Contour plot of the Gaussian mixture model in  $S^2$

*Contour plot of the Gaussian mixture model in  $S^2$*

---

**Description**

Contour plot of the Gaussian mixture model in  $S^2$ .

**Usage**

```
mix.compnorm.contour(mod, type = "alr", n = 100, x = NULL, cont.line = FALSE)
```

**Arguments**

mod	An object containing the output of a <code>mix.compnorm</code> model.
type	The type of transformation used, either the additive log-ratio ("alr"), the isometric log-ratio ("ilr") or the pivot coordinate ("pivot") transformation.
n	The number of grid points to consider over which the density is calculated.
x	A matrix with the compositional data.
cont.line	Do you want the contour lines to appear? If yes, set this TRUE.

**Details**

The contour plot of a Gaussian mixture model is plotted. For this you need the (fitted) model.

**Value**

A ternary plot with the data and the contour lines of the fitted Gaussian mixture model.

**Author(s)**

Michail Tsagris and Christos Adam.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Christos Adam <pada4m4@gmail.com>.

**References**

Ryan P. Browne, Aisha ElSherbiny and Paul D. McNicholas (2015). R package mixture: Mixture Models for Clustering and Classification

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

**See Also**

[mix.compnorm](#), [bic.mixcompnorm](#), [diri.contour](#)

**Examples**

```
x <- as.matrix(iris[, 1:3])
x <- x / rowSums(x)
mod <- mix.compnorm(x, 3, model = "EII")
mix.compnorm.contour(mod, "alr")
```

---

Contour plot of the generalised Dirichlet distribution in  $S^2$

*Contour plot of the generalised Dirichlet distribution in  $S^2$*

---

**Description**

Contour plot of the generalised Dirichlet distribution in  $S^2$ .

**Usage**

```
gendiri.contour(a, b, n = 100, x = NULL, cont.line = FALSE)
```

**Arguments**

a	A vector with three elements corresponding to the 3 (estimated) shape parameter values.
b	A vector with three elements corresponding to the 3 (estimated) scale parameter values.
n	The number of grid points to consider over which the density is calculated.
x	This is either NULL (no data) or contains a 3 column matrix with compositional data.
cont.line	Do you want the contour lines to appear? If yes, set this TRUE.

**Details**

The user can plot only the contour lines of a Dirichlet with a given vector of parameters, or can also add the relevant data should he/she wish to.

**Value**

A ternary diagram with the points and the Dirichlet contour lines.

**Author(s)**

Michail Tsagris and Christos Adam.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Christos Adam <pada4m4@gmail.com>.

**References**

Ng Kai Wang, Guo-Liang Tian and Man-Lai Tang (2011). Dirichlet and related distributions: Theory, methods and applications. John Wiley & Sons.

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

**See Also**

[diri.contour](#), [mixdiri.contour](#), [compnorm.contour](#), [comp.kerncontour](#), [mix.compnorm.contour](#)

**Examples**

```
x <- as.matrix( iris[, 1:3] )
x <- x / rowSums(x)
gendiri.contour( a = c(3, 4, 2), b = c(1, 2, 3) )
```

---

Contour plot of the kernel density estimate in  $S^2$

*Contour plot of the kernel density estimate in  $S^2$*

---

**Description**

Contour plot of the kernel density estimate in  $S^2$ .

**Usage**

```
comp.kerncontour(x, type = "alr", n = 50, cont.line = FALSE)
```



**Arguments**

<code>x</code>	A matrix with the compositional data. It has to be a 3 column matrix.
<code>type</code>	This is either "alr" or "ilr", corresponding to the additive and the isometric log-ratio transformation respectively.
<code>n</code>	The number of grid points to consider, over which the density is calculated.
<code>cont.line</code>	Do you want the contour lines to appear? If yes, set this TRUE.

**Details**

The alr or the ilr transformation are applied to the compositional data. Then, the optimal bandwidth using maximum likelihood cross-validation is chosen. The multivariate normal kernel density is calculated for a grid of points. Those points are the points on the 2-dimensional simplex. Finally the contours are plotted.

**Value**

A ternary diagram with the points and the kernel contour lines.

**Author(s)**

Michail Tsagris and Christos Adam.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Christos Adam <pada4m4@gmail.com>.

**References**

M.P. Wand and M.C. Jones (1995). Kernel smoothing, CrC Press.

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

**See Also**

[diri.contour](#), [mix.compnorm.contour](#), [bivt.contour](#), [compnorm.contour](#)

**Examples**

```
x <- as.matrix(iris[, 1:3])
x <- x / rowSums(x)
comp.kerncontour(x, type = "alr", n = 20)
comp.kerncontour(x, type = "ilr", n = 20)
```

---

Contour plot of the normal distribution in  $S^2$

*Contour plot of the normal distribution in  $S^2$*

---

## Description

Contour plot of the normal distribution in  $S^2$ .

## Usage

```
compnorm.contour(m, s, type = "alr", n = 100, x = NULL, cont.line = FALSE)
```

## Arguments

<code>m</code>	The mean vector.
<code>s</code>	The covariance matrix.
<code>type</code>	The type of transformation used, either the additive log-ratio ("alr"), the isometric log-ratio ("ilr") or the pivot coordinate ("pivot") transformation.
<code>n</code>	The number of grid points to consider over which the density is calculated.
<code>x</code>	This is either NULL (no data) or contains a 3 column matrix with compositional data.
<code>cont.line</code>	Do you want the contour lines to appear? If yes, set this TRUE.

## Details

The alr or the ilr transformation is applied to the compositional data at first. Then for a grid of points within the 2-dimensional simplex the bivariate normal density is calculated and the contours are plotted along with the points.

## Value

A ternary diagram with the points (if `appear = TRUE`) and the bivariate normal contour lines.

## Author(s)

Michail Tsagris and Christos Adam.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Christos Adam <pada4m4@gmail.com>.

## See Also

[diri.contour](#), [mix.compnorm.contour](#), [bivt.contour](#), [skewnorm.contour](#)

**Examples**

```
x <- as.matrix(iris[, 1:3])
x <- x / rowSums(x)
y <- Compositional::alr(x)
m <- colMeans(y)
s <- cov(y)
compnorm.contour(m, s)
```

---

Contour plot of the skew skew-normal distribution in  $S^2$

*Contour plot of the skew skew-normal distribution in  $S^2$*

---

**Description**

Contour plot of the skew skew-normal distribution in  $S^2$ .

**Usage**

```
skewnrm.contour(x, type = "alr", n = 100, appear = TRUE, cont.line = FALSE)
```

**Arguments**

x	A matrix with the compositional data. It has to be a 3 column matrix.
type	This is either "alr" or "ilr", corresponding to the additive and the isometric log-ratio transformation respectively.
n	The number of grid points to consider over which the density is calculated.
appear	Should the available data appear on the ternary plot (TRUE) or not (FALSE)?
cont.line	Do you want the contour lines to appear? If yes, set this TRUE.

**Details**

The alr or the ilr transformation is applied to the compositional data at first. Then for a grid of points within the 2-dimensional simplex the bivariate skew skew-normal density is calculated and the contours are plotted along with the points.

**Value**

A ternary diagram with the points (if appear = TRUE) and the bivariate skew skew-normal contour lines.

**Author(s)**

Michail Tsagris and Christos Adam.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Christos Adam <pada4m4@gmail.com>.

**References**

- Azzalini A. and Valle A. D. (1996). The multivariate skew-skewnormal distribution. *Biometrika* 83(4):715-726.
- Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

**See Also**

[diri.contour](#), [mix.compnorm.contour](#), [bivt.contour](#), [compnorm.contour](#)

**Examples**

```
x <- as.matrix(iris[51:100, 1:3])
x <- x / rowSums(x)
skewnorm.contour(x)
```

---

Contour plot of the  $t$  distribution in  $S^2$   
*Contour plot of the  $t$  distribution in  $S^2$*

---

**Description**

Contour plot of the  $t$  distribution in  $S^2$ .

**Usage**

```
bivt.contour(x, type = "alr", n = 100, appear = TRUE, cont.line = FALSE)
```

**Arguments**

<code>x</code>	A matrix with compositional data. It has to be a 3 column matrix.
<code>type</code>	This is either "alr" or "ilr", corresponding to the additive and the isometric log-ratio transformation respectively.
<code>n</code>	The number of grid points to consider over which the density is calculated.
<code>appear</code>	Should the available data appear on the ternary plot (TRUE) or not (FALSE)?
<code>cont.line</code>	Do you want the contour lines to appear? If yes, set this TRUE.

**Details**

The alr or the ilr transformation is applied to the compositional data at first and the location, scatter and degrees of freedom of the bivariate  $t$  distribution are computed. Then for a grid of points within the 2-dimensional simplex the bivariate  $t$  density is calculated and the contours are plotted along with the points.

**Value**

A ternary diagram with the points (if `appear = TRUE`) and the bivariate  $t$  contour lines.

**Author(s)**

Michail Tsagris and Christos Adam.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Christos Adam <pada4m4@gmail.com>.

**References**

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

**See Also**

[diri.contour](#), [mix.compnorm.contour](#), [compnorm.contour](#), [skewnorm.contour](#)

**Examples**

```
x <- as.matrix( iris[, 1:3] )
x <- x / rowSums(x)
bivt.contour(x)
bivt.contour(x, type = "ilr")
```

---

Cross validation for some compositional regression models

*Cross validation for some compositional regression models*

---

**Description**

Cross validation for some compositional regression models.

**Usage**

```
cv.comp.reg(y, x, type = "comp.reg", nfolds = 10, folds = NULL, seed = NULL)
```

**Arguments**

y	A matrix with compositional data. Zero values are allowed for some regression models.
x	The predictor variable(s).
type	This can be one of the following: "comp.reg", "robust", "kl.compreg", "js.compreg", "diri.reg" or "zadr".
nfolds	The number of folds to be used. This is taken into consideration only if the folds argument is not supplied.
folds	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.
seed	If seed is TRUE the results will always be the same.

**Details**

A k-fold cross validation for a compositional regression model is performed.

**Value**

A list including:

runtime	The runtime of the cross-validation procedure.
kl	The Kullback-Leibler divergences for all runs.
js	The Jensen-Shannon divergences for all runs.
perf	The average Kullback-Leibler divergence and average Jensen-Shannon divergence.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**See Also**

[comp.reg](#), [kl.compreg](#), [compppr.tune](#), [aknreg.tune](#)

**Examples**

```
y <- as.matrix( iris[, 1:3] )
y <- y / rowSums(y)
x <- iris[, 4]
mod <- cv.comp.reg(y, x)
```

---

Cross validation for the alpha-k-NN regression with compositional predictor variables

*Cross validation for the  $\alpha$ -k-NN regression with compositional predictor variables*

---

**Description**

Cross validation for the  $\alpha$ -k-NN regression with compositional predictor variables.

**Usage**

```
alfaknreg.tune(y, x, a = seq(-1, 1, by = 0.1), k = 2:10, nfolds = 10,
apostasi = "euclidean", method = "average", folds = NULL, seed = NULL, graph = FALSE)
```

**Arguments**

y	The response variable, a numerical vector.
x	A matrix with the available compositional data. Zeros are allowed.
a	A vector with a grid of values of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ the isometric log-ratio transformation is applied.
k	The number of nearest neighbours to consider. It can be a single number or a vector.
nfolds	The number of folds. Set to 10 by default.
apostasi	The type of distance to use, either "euclidean" or "manhattan".
method	If you want to take the average of the responses of the k closest observations, type "average". For the median, type "median" and for the harmonic mean, type "harmonic".
folds	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.
seed	If seed is TRUE the results will always be the same.
graph	If graph is TRUE (default value) a filled contour plot will appear.

**Details**

A k-fold cross validation for the  $\alpha$ -k-NN regression for compositional response data is performed.

**Value**

A list including:

mspe	The mean square error of prediction.
performance	The minimum mean square error of prediction.
opt_a	The optimal value of $\alpha$ .
opt_k	The optimal value of k.
runtime	The runtime of the cross-validation procedure.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Tsagris M., Alenazi A. and Stewart C. (2023). Flexible non-parametric regression models for compositional response data with zeros. *Statistics and Computing*, 33(106).

<https://link.springer.com/article/10.1007/s11222-023-10277-5>

**See Also**

[alfa.rda](#), [alfa.fda](#)

**Examples**

```
library(MASS)
x <- as.matrix(fgl[, 2:9])
x <- x / rowSums(x)
y <- fgl[, 1]
mod <- alfaknnreg.tune(y, x, a = seq(0.2, 0.4, by = 0.1), k = 2:4, nfolds = 5)
```

---

Cross validation for the alpha-k-NN regression with compositional response data

*Cross validation for the  $\alpha$ -k-NN regression with compositional response data*

---

**Description**

Cross validation for the  $\alpha$ -k-NN regression with compositional response data.

**Usage**

```
aknnreg.tune(y, x, a = seq(0.1, 1, by = 0.1), k = 2:10, apostasi = "euclidean",
nfolds = 10, folds = NULL, seed = NULL, rann = FALSE)
```

**Arguments**

y	A matrix with the compositional response data. Zeros are allowed.
x	A matrix with the available predictor variables.
a	A vector with a grid of values of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ the isometric log-ratio transformation is applied.
k	The number of nearest neighbours to consider. It can be a single number or a vector.
apostasi	The type of distance to use, either "euclidean" or "manhattan".
nfolds	The number of folds. Set to 10 by default.
folds	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.
seed	You can specify your own seed number here or leave it NULL.
rann	If you have large scale datasets and want a faster k-NN search, you can use kd-trees implemented in the R package "Rnanoflann". In this case you must set this argument equal to TRUE. Note however, that in this case, the only available distance is by default "euclidean".

**Details**

A k-fold cross validation for the  $\alpha$ -k-NN regression for compositional response data is performed.



**Value**

A list including:

kl	The Kullback-Leibler divergence for all combinations of $\alpha$ and $k$ .
js	The Jensen-Shannon divergence for all combinations of $\alpha$ and $k$ .
klmin	The minimum Kullback-Leibler divergence.
jsmin	The minimum Jensen-Shannon divergence.
kl.alpha	The optimal $\alpha$ that leads to the minimum Kullback-Leibler divergence.
kl.k	The optimal $k$ that leads to the minimum Kullback-Leibler divergence.
js.alpha	The optimal $\alpha$ that leads to the minimum Jensen-Shannon divergence.
js.k	The optimal $k$ that leads to the minimum Jensen-Shannon divergence.
runtime	The runtime of the cross-validation procedure.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Tsagris M., Alenazi A. and Stewart C. (2023). Flexible non-parametric regression models for compositional response data with zeros. *Statistics and Computing*, 33(106).

<https://link.springer.com/article/10.1007/s11222-023-10277-5>

**See Also**

[aknn.reg](#), [akernreg.tune](#), [akern.reg](#), [alfa.rda](#), [alfa.fda](#)

**Examples**

```
y <- as.matrix( iris[, 1:3] )
y <- y / rowSums(y)
x <- iris[, 4]
mod <- aknnreg.tune(y, x, a = c(0.4, 0.6), k = 2:4, nolds = 5)
```

---

Cross validation for the alpha-kernel regression with compositional response data

*Cross validation for the  $\alpha$ -kernel regression with compositional response data*

---

**Description**

Cross validation for the  $\alpha$ -kernel regression with compositional response data.

**Usage**

```
akernreg.tune(y, x, a = seq(0.1, 1, by = 0.1), h = seq(0.1, 1, length = 10),
  type = "gauss", n folds = 10, folds = NULL, seed = NULL)
```

**Arguments**

y	A matrix with the compositional response data. Zeros are allowed.
x	A matrix with the available predictor variables.
a	A vector with a grid of values of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ the isometric log-ratio transformation is applied.
h	A vector with the bandwidth value(s) to consider.
type	The type of kernel to use, "gauss" or "laplace".
n folds	The number of folds. Set to 10 by default.
folds	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.
seed	You can specify your own seed number here or leave it NULL.

**Details**

A k-fold cross validation for the  $\alpha$ -kernel regression for compositional response data is performed.

**Value**

A list including:

kl	The Kullback-Leibler divergence for all combinations of $\alpha$ and $h$ .
js	The Jensen-Shannon divergence for all combinations of $\alpha$ and $h$ .
klmin	The minimum Kullback-Leibler divergence.
jsmin	The minimum Jensen-Shannon divergence.
kl.alpha	The optimal $\alpha$ that leads to the minimum Kullback-Leibler divergence.
kl.h	The optimal $h$ that leads to the minimum Kullback-Leibler divergence.
js.alpha	The optimal $\alpha$ that leads to the minimum Jensen-Shannon divergence.
js.h	The optimal $h$ that leads to the minimum Jensen-Shannon divergence.
runtime	The runtime of the cross-validation procedure.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Tsagris M., Alenazi A. and Stewart C. (2023). Flexible non-parametric regression models for compositional response data with zeros. *Statistics and Computing*, 33(106).

<https://link.springer.com/article/10.1007/s11222-023-10277-5>

**See Also**

[akern.reg](#), [aknreg.tune](#), [aknn.reg](#), [alfa.rda](#), [alfa.fda](#)

**Examples**

```
y <- as.matrix( iris[, 1:3] )
y <- y / rowSums(y)
x <- iris[, 4]
mod <- akernreg.tune(y, x, a = c(0.4, 0.6), h = c(0.1, 0.2), nfolds = 5)
```

---

Cross validation for the kernel regression with Euclidean response data

*Cross validation for the kernel regression with Euclidean response data*

---

**Description**

Cross validation for the kernel regression with Euclidean response data.

**Usage**

```
kernreg.tune(y, x, h = seq(0.1, 1, length = 10), type = "gauss",
nfolds = 10, folds = NULL, seed = NULL, graph = FALSE, ncores = 1)
```

**Arguments**

<code>y</code>	A matrix or a vector with the Euclidean response.
<code>x</code>	A matrix with the available predictor variables.
<code>h</code>	A vector with the bandwidth value(s) $h$ to consider.
<code>type</code>	The type of kernel to use, "gauss" or "laplace".
<code>nfolds</code>	The number of folds. Set to 10 by default.
<code>folds</code>	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.
<code>seed</code>	You can specify your own seed number here or leave it NULL.
<code>graph</code>	If graph is TRUE (default value) a plot will appear.
<code>ncores</code>	The number of cores to use. Default value is 1.

**Details**

A k-fold cross validation for the kernel regression with a euclidean response is performed.

## Value

A list including:

mspe	The mean squared prediction error (MSPE) for each fold and value of $h$ .
h	The optimal $h$ that leads to the minimum MSPE.
performance	The minimum MSPE.
runtime	The runtime of the cross-validation procedure.

## Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

## References

Wand M. P. and Jones M. C. (1994). Kernel smoothing. CRC press.

## See Also

[kern.reg](#), [aknreg.tune](#), [aknn.reg](#)

## Examples

```
y <- iris[, 1]
x <- iris[, 2:4]
mod <- kernreg.tune(y, x, h = c(0.1, 0.2, 0.3) )
```

---

Cross validation for the regularised and flexible discriminant analysis with compositional data using the alpha-transformation

*Cross validation for the regularised and flexible discriminant analysis with compositional data using the  $\alpha$ -transformation*

---

## Description

Cross validation for the regularised and flexible discriminant analysis with compositional data using the  $\alpha$ -transformation.

## Usage

```
alfarda.tune(x, ina, a = seq(-1, 1, by = 0.1), nfolds = 10,
gam = seq(0, 1, by = 0.1), del = seq(0, 1, by = 0.1),
ncores = 1, folds = NULL, stratified = TRUE, seed = NULL)
```

```
alfafda.tune(x, ina, a = seq(-1, 1, by = 0.1), nfolds = 10,
folds = NULL, stratified = TRUE, seed = NULL, graph = FALSE)
```

## Arguments

x	A matrix with the available compositional data. Zeros are allowed.
ina	A group indicator variable for the available data.
a	A vector with a grid of values of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ the isometric log-ratio transformation is applied.
nfolds	The number of folds. Set to 10 by default.
gam	A vector of values between 0 and 1. It is the weight of the pooled covariance and the diagonal matrix.
del	A vector of values between 0 and 1. It is the weight of the LDA and QDA.
ncores	The number of cores to use. If it is more than 1 parallel computing is performed. It is advisable to use it if you have many observations and or many variables, otherwise it will slow down the process.
fold	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.
stratified	Do you want the folds to be created in a stratified way? TRUE or FALSE.
seed	You can specify your own seed number here or leave it NULL.
graph	If graph is TRUE (default value) a plot will appear.

## Details

A k-fold cross validation is performed.

## Value

For the `alfa.rda` a list including:

res	The estimated optimal rate and the best values of $\alpha$ , $\gamma$ and $\delta$ .
percent	For the best value of $\alpha$ the averaged over all folds best rates of correct classification. It is a matrix, where rows correspond to the $\gamma$ values and columns correspond to $\delta$ values.
se	The estimated standard errors of the "percent" matrix.
runtime	The runtime of the cross-validation procedure.

For the `alfa.fda` a graph (if requested) with the estimated performance for each value of  $\alpha$  and a list including:

per	The performance of the fda in each fold for each value of $\alpha$ .
performance	The average performance for each value of $\alpha$ .
opt_a	The optimal value of $\alpha$ .
runtime	The runtime of the cross-validation procedure.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Giorgos Athineou <gioathineou@gmail.com>.

**References**

Friedman Jerome, Trevor Hastie and Robert Tibshirani (2009). The elements of statistical learning, 2nd edition. Springer, Berlin

Tsagris M.T., Preston S. and Wood A.T.A. (2016). Improved classification for compositional data using the  $\alpha$ -transformation. *Journal of Classification*, 33(2):243-261.

Hastie, Tibshirani and Buja (1994). Flexible Discriminant Analysis by Optimal Scoring. *Journal of the American Statistical Association*, 89(428):1255-1270.

**See Also**

[alfa.rda](#), [alfanb.tune](#), [cv.dda](#), [compknn.tune](#) [cv.compnb](#)

**Examples**

```
library(MASS)
x <- as.matrix(fg1[, 2:9])
x <- x / rowSums(x)
ina <- fg1[, 10]
moda <- alfarda.tune(x, ina, a = seq(0.7, 1, by = 0.1), nfolds = 10,
gam = seq(0.1, 0.3, by = 0.1), del = seq(0.1, 0.3, by = 0.1) )
```

---

Cross validation for the ridge regression

*Cross validation for the ridge regression*

---

**Description**

Cross validation for the ridge regression is performed. There is an option for the GCV criterion which is automatic.

**Usage**

```
ridge.tune(y, x, nfolds = 10, lambda = seq(0, 2, by = 0.1), folds = NULL,
ncores = 1, seed = NULL, graph = FALSE)
```

**Arguments**

y	A numeric vector containing the values of the target variable. If the values are proportions or percentages, i.e. strictly within 0 and 1 they are mapped into R using the logit transformation.
x	A numeric matrix containing the variables.
nfolds	The number of folds in the cross validation.
lambda	A vector with the a grid of values of $\lambda$ to be used.
folds	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.
ncores	The number of cores to use. If it is more than 1 parallel computing is performed.
seed	You can specify your own seed number here or leave it NULL.
graph	If graph is set to TRUE the performances for each fold as a function of the $\lambda$ values will appear.

**Details**

A k-fold cross validation is performed. This function is used by [alfaridge.tune](#).

**Value**

A list including:

msep	The performance of the ridge regression for every fold.
mspe	The values of the mean prediction error for each value of $\lambda$ .
lambda	The value of $\lambda$ which corresponds to the minimum MSPE.
performance	The minimum MSPE.
runtime	The time required by the cross-validation procedure.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Giorgos Athineou <[gioathineou@gmail.com](mailto:gioathineou@gmail.com)> and Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

**References**

Hoerl A.E. and R.W. Kennard (1970). Ridge regression: Biased estimation for nonorthogonal problems. *Technometrics*, 12(1):55-67.

Brown P. J. (1994). *Measurement, Regression and Calibration*. Oxford Science Publications.

**See Also**

[ridge.reg](#), [alfaridge.tune](#)

## Examples

```
y <- as.vector(iris[, 1])
x <- as.matrix(iris[, 2:4])
ridge.tune( y, x, nfolds = 10, lambda = seq(0, 2, by = 0.1), graph = TRUE )
```

---

Cross validation for the ridge regression with compositional data  
as predictor using the alpha-transformation

*Cross validation for the ridge regression with compositional data as  
predictor using the  $\alpha$ -transformation*

---

## Description

Cross validation for the ridge regression is performed. There is an option for the GCV criterion which is automatic. The predictor variables are compositional data and the  $\alpha$ -transformation is applied first.

## Usage

```
alfaridge.tune(y, x, nfolds = 10, a = seq(-1, 1, by = 0.1),
lambda = seq(0, 2, by = 0.1), folds = NULL, ncores = 1,
graph = TRUE, col.nu = 15, seed = NULL)
```

## Arguments

y	A numeric vector containing the values of the target variable. If the values are proportions or percentages, i.e. strictly within 0 and 1 they are mapped into R using the logit transformation.
x	A numeric matrix containing the compositional data, i.e. the predictor variables. Zero values are allowed.
nfolds	The number of folds in the cross validation.
a	A vector with the a grid of values of $\alpha$ to be used.
lambda	A vector with the a grid of values of $\lambda$ to be used.
folds	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.
ncores	The number of cores to use. If it is more than 1 parallel computing is performed. It is advisable to use it if you have many observations and or many variables, otherwise it will slow down th process.
graph	If graph is TRUE (default value) a filled contour plot will appear.
col.nu	A number parameter for the filled contour plot, taken into account only if graph is TRUE.
seed	You can specify your own seed number here or leave it NULL.



## Details

A k-fold cross validation is performed.

## Value

If graph is TRUE a field contour a filled contour will appear. A list including:

mspe	The MSPE where rows correspond to the $\alpha$ values and the columns to the number of principal components.
best.par	The best pair of $\alpha$ and $\lambda$ .
performance	The minimum mean squared error of prediction.
runtime	The run time of the cross-validation procedure.

## Author(s)

Michail Tsagris.

R implementation and documentation: Giorgos Athineou <gioathineou@gmail.com> and Michail Tsagris <mtsagris@uoc.gr>.

## References

Hoerl A.E. and R.W. Kennard (1970). Ridge regression: Biased estimation for nonorthogonal problems. *Technometrics*, 12(1):55-67.

Brown P. J. (1994). *Measurement, Regression and Calibration*. Oxford Science Publications.

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In *Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain*. <https://arxiv.org/pdf/1106.1451.pdf>

## See Also

[alfa.ridge](#), [ridge.tune](#)

## Examples

```
library(MASS)
y <- as.vector(fgl[, 1])
x <- as.matrix(fgl[, 2:9])
x <- x / rowSums(x)
alfaridge.tune( y, x, nfolds = 10, a = seq(0.1, 1, by = 0.1),
lambda = seq(0, 1, by = 0.1) )
```

---

Cross validation for the TFLR model

*Cross validation for the TFLR model*

---

### **Description**

Cross validation for the TFLR model.

### **Usage**

```
cv.tflr(y, x, nfolds = 10, folds = NULL, seed = NULL)
```

### **Arguments**

y	A matrix with compositional response data. Zero values are allowed.
x	A matrix with compositional predictors. Zero values are allowed.
nfolds	The number of folds to be used. This is taken into consideration only if the folds argument is not supplied.
folds	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.
seed	If seed is TRUE the results will always be the same.

### **Details**

A k-fold cross validation for the transformation-free linear regression for compositional responses and predictors is performed.

### **Value**

A list including:

runtime	The runtime of the cross-validation procedure.
kl	The Kullback-Leibler divergences for all runs.
js	The Jensen-Shannon divergences for all runs.
perf	The average Kullback-Leibler divergence and average Jensen-Shannon divergence.

### **Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

### **References**

Fiksel J., Zeger S. and Datta A. (2022). A transformation-free linear regression for compositional outcomes and predictors. *Biometrics*, 78(3): 974–987.

Tsagris. M. (2024). Constrained least squares simplicial-simplicial regression. <https://arxiv.org/pdf/2403.19835.pdf>

**See Also**

[tflr](#), [cv.scls](#), [klalfapcr.tune](#)

**Examples**

```
library(MASS)
y <- rdirich(100, runif(3, 1, 3))
x <- as.matrix(fgl[1:100, 2:9])
x <- x / rowSums(x)
mod <- cv.tflr(y, x)
mod
```

---

Cross-validation for LASSO with compositional predictors using the alpha-transformation

*Cross-validation for LASSO with compositional predictors using the alpha-transformation*

---

**Description**

Cross-validation for LASSO with compositional predictors using the *alpha*-transformation.

**Usage**

```
alfalasso.tune(y, x, a = seq(-1, 1, by = 0.1), model = "gaussian", lambda = NULL,
  type.measure = "mse", nfolds = 10, folds = NULL, stratified = FALSE)
```

**Arguments**

- |                     |   |
|---------------------|---|
| <code>y</code>      | A numerical vector or a matrix for multinomial logistic regression.   |
| <code>x</code>      | A numerical matrix containing the predictor variables, compositional data, where zero values are allowed..  |
| <code>a</code>      | A vector with a grid of values of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ the isometric log-ratio transformation is applied.   |
| <code>model</code>  | The type of the regression model, "gaussian", "binomial", "poisson", "multinomial", or "mgaussian".   |
| <code>lambda</code> | <b>This information is copied from the package <code>glmnet</code>.</b> A user supplied lambda sequence. Typical usage is to have the program compute its own lambda sequence based on <code>nlambda</code> and <code>lambda.min.ratio</code> . Supplying a value of lambda overrides this. <b>WARNING:</b> use with care. Avoid supplying a single value for lambda (for predictions after CV use <code>predict()</code> instead). Supply instead a decreasing sequence of lambda values. <code>glmnet</code> relies on its warm starts for speed, and its often faster to fit a whole path than compute a single fit. |

type.measure	<b>This information is taken from the package glmnet.</b> The loss function to use for cross-validation. For gaussian models this can be "mse", "deviance" for logistic and poisson regression, "class" applies to binomial and multinomial logistic regression only, and gives misclassification error. "auc" is for two-class logistic regression only, and gives The area under the ROC curve. "mse" or "mae" (mean absolute error) can be used by all models.
nfolds	The number of folds. Set to 10 by default.
folds	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.
stratified	Do you want the folds to be created in a stratified way? TRUE or FALSE.

### Details

The function uses the glmnet package to perform LASSO penalised regression. For more details see the function in that package.

### Value

A matrix with two columns and number of rows equal to the number of  $\alpha$  values used. Each row contains, the optimal value of the  $\lambda$  penalty parameter for the LASSO and the optimal value of the loss function, for each value of  $\alpha$ .

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

### References

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

Friedman, J., Hastie, T. and Tibshirani, R. (2010) Regularization Paths for Generalized Linear Models via Coordinate Descent. Journal of Statistical Software, Vol. 33(1), 1–22.

### See Also

[alfa.lasso](#), [cv.lasso.klcompreg](#), [lasso.compreg](#), [alfa.knn.reg](#)

### Examples

```
y <- iris[, 1]
x <- rdiri(150, runif(20, 2, 5) )
mod <- alfa.lasso.tune( y, x, a = c(0.2, 0.5, 1) )
```

---

Cross-validation for the alpha-SCLS model  
*Cross-validation for the alpha-SCLS model*

---

**Description**

Cross-validation for the *alpha*-SCLS model.

**Usage**

```
cv.ascls(y, x, a = seq(0.1, 1, by = 0.1), nfolds = 10, folds = NULL, seed = NULL)
```

**Arguments**

<code>y</code>	A numerical matrix with the simplicial response data. Zero values are allowed.
<code>x</code>	A matrix with the simplicial predictor variables. Zero values are allowed.
<code>a</code>	A vector or a single number of values of the $\alpha$ -parameter. This has to be different from zero, and it can take negative values if there are no zeros in the simplicial response ( <code>y</code> ).
<code>nfolds</code>	The number of folds for the K-fold cross validation, set to 10 by default.
<code>folds</code>	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.
<code>seed</code>	You can specify your own seed number here or leave it NULL.

**Details**

The K-fold cross validation is performed in order to select the optimal value for  $\alpha$  of the  $\alpha$ -SCLS model.

**Value**

A list including:

<code>runtime</code>	The runtime of the cross-validation procedure.
<code>kl</code>	The Kullback-Leibler divergence for every value of $\alpha$ .
<code>js</code>	The Jensen-Shannon divergence for every value of $\alpha$ .

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Tsagris, M. (2024). Constrained least squares simplicial-simplicial regression. <https://arxiv.org/pdf/2403.19835.pdf>

**See Also**

[ascls](#), [cv.atflr](#)

**Examples**

```
library(MASS)
y <- rdirichlet(214, runif(4, 1, 3) )
x <- as.matrix( fgl[, 2:9] )
mod <- cv.ascls(y, x, nfold = 5)
```

---

Cross-validation for the *alpha-TFLR* model

*Cross-validation for the *alpha-TFLR* model*

---

**Description**

Cross-validation for the *alpha-TFLR* model.

**Usage**

```
cv.atflr(y, x, a = seq(0.1, 1, by = 0.1), nfold = 10, folds = NULL, seed = NULL)
```

**Arguments**

<code>y</code>	A numerical matrix with the simplicial response data. Zero values are allowed.
<code>x</code>	A matrix with the simplicial predictor variables. Zero values are allowed.
<code>a</code>	A vector or a single number of values of the $\alpha$ -parameter. This has to be different from zero, and it can take negative values if there are no zeros in the simplicial response ( <code>y</code> ).
<code>nfold</code>	The number of folds for the K-fold cross validation, set to 10 by default.
<code>folds</code>	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.
<code>seed</code>	You can specify your own seed number here or leave it NULL.

**Details**

The K-fold cross validation is performed in order to select the optimal value for  $\alpha$  of the *alpha-TFLR* model.

**Value**

A list including:

<code>runtime</code>	The runtime of the cross-validation procedure.
<code>kl</code>	The Kullback-Leibler divergence for every value of $\alpha$ .
<code>js</code>	The Jensen-Shannon divergence for every value of $\alpha$ .

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Fiksel J., Zeger S. and Datta A. (2022). A transformation-free linear regression for compositional outcomes and predictors. *Biometrics*, 78(3): 974–987.

Tsagris. M. (2024). Constrained least squares simplicial-simplicial regression. <https://arxiv.org/pdf/2403.19835.pdf>

**See Also**

[atflr](#), [cv.ascls](#)

**Examples**

```
library(MASS)
y <- rdiri( 214, runif(4, 1, 3) )
x <- as.matrix( fgl[, 2:9] )
mod <- cv.ascls(y, x, nfolds = 2, a = c(0.5, 1))
```

---

Cross-validation for the Dirichlet discriminant analysis

*Cross-validation for the Dirichlet discriminant analysis*

---

**Description**

Cross-validation for the Dirichlet discriminant analysis.

**Usage**

```
cv.dda(x, ina, nfolds = 10, folds = NULL, stratified = TRUE, seed = NULL)
```

**Arguments**

<code>x</code>	A matrix with the available data, the predictor variables.
<code>ina</code>	A vector of data. The response variable, which is categorical (factor is acceptable).
<code>folds</code>	A list with the indices of the folds.
<code>nfolds</code>	The number of folds to be used. This is taken into consideration only if "folds" is NULL.
<code>stratified</code>	Do you want the folds to be selected using stratified random sampling? This preserves the analogy of the samples of each group. Make this TRUE if you wish.
<code>seed</code>	If you set this to TRUE, the same folds will be created every time.

**Details**

This function estimates the performance of the Dirichlet discriminant analysis via k-fold cross-validation.

**Value**

A list including:

percent	The percentage of correct classification
runtime	The duration of the cross-validation procedure.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

**References**

Friedman J., Hastie T. and Tibshirani R. (2017). The elements of statistical learning. New York: Springer.

Thomas P. Minka (2003). Estimating a Dirichlet distribution. <http://research.microsoft.com/en-us/um/people/minka/papers/dirichlet/minka-dirichlet.pdf>

**See Also**

[dda](#), [alfanb.tune](#), [alfarda.tune](#), [compknn.tune](#), [cv.comprnb](#)

**Examples**

```
x <- as.matrix(iris[, 1:4])
x <- x / rowSums(x)
mod <- cv.dda(x, ina = iris[, 5] )
```

---

Cross-validation for the LASSO Kullback-Leibler divergence based regression

*Cross-validation for the LASSO Kullback-Leibler divergence based regression*

---

**Description**

Cross-validation for the LASSO Kullback-Leibler divergence based regression.

**Usage**

```
cv.lasso.klcompreg(y, x, alpha = 1, type = "grouped", nfolds = 10,
folds = NULL, seed = NULL, graph = FALSE)
```



**Arguments**

y	A numerical matrix with compositional data with or without zeros.
x	A matrix with the predictor variables.
alpha	The elastic net mixing parameter, with $0 \leq \alpha \leq 1$ . The penalty is defined as a weighted combination of the ridge and of the Lasso regression. When $\alpha = 1$ LASSO is applied, while $\alpha = 0$ yields the ridge regression.
type	<b>This information is copied from the package glmnet.</b> If "grouped" then a grouped lasso penalty is used on the multinomial coefficients for a variable. This ensures they are all in our out together. The default in our case is "grouped".
nfolds	The number of folds for the K-fold cross validation, set to 10 by default.
folds	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.
seed	You can specify your own seed number here or leave it NULL.
graph	If graph is TRUE (default value) a filled contour plot will appear.

**Details**

The K-fold cross validation is performed in order to select the optimal value for  $\lambda$ , the penalty parameter in LASSO.

**Value**

The outcome is the same as in the R package glmnet. The extra addition is that if "graph = TRUE", then the plot of the cross-validated object is returned. The contains the logarithm of  $\lambda$  and the deviance. The numbers on top of the figure show the number of set of coefficients for each component, that are not zero.

**Author(s)**

Michail Tsagris and Abdulaziz Alenazi.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Abdulaziz Alenazi <a.alenazi@nbu.edu.sa>.

**References**

Alenazi, A. A. (2022). f-divergence regression models for compositional data. *Pakistan Journal of Statistics and Operation Research*, 18(4): 867–882.

Friedman, J., Hastie, T. and Tibshirani, R. (2010) Regularization Paths for Generalized Linear Models via Coordinate Descent. *Journal of Statistical Software*, Vol. 33(1), 1-22.

**See Also**

[lasso.klcompreg](#), [lassocoeff.plot](#), [lasso.compreg](#), [cv.lasso.compreg](#), [kl.compreg](#)

**Examples**

```
library(MASS)
y <- rdir( 214, runif(4, 1, 3) )
x <- as.matrix( fgl[, 2:9] )
mod <- cv.lasso.klcompreg(y, x)
```

---

Cross-validation for the LASSO log-ratio regression with compositional response

*Cross-validation for the LASSO log-ratio regression with compositional response*

---

**Description**

Cross-validation for the LASSO log-ratio regression with compositional response.

**Usage**

```
cv.lasso.compreg(y, x, alpha = 1, nolds = 10,
folds = NULL, seed = NULL, graph = FALSE)
```

**Arguments**

y	A numerical matrix with compositional data. Zero values are not allowed as the additive log-ratio transformation ( <a href="#">alr</a> ) is applied to the compositional response prior to implementing the LASSO algorithm.
x	A matrix with the predictor variables.
alpha	The elastic net mixing parameter, with $0 \leq \alpha \leq 1$ . The penalty is defined as a weighted combination of the ridge and of the Lasso regression. When $\alpha = 1$ LASSO is applied, while $\alpha = 0$ yields the ridge regression.
nolds	The number of folds for the K-fold cross validation, set to 10 by default.
folds	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.
seed	You can specify your own seed number here or leave it NULL.
graph	If graph is TRUE (default value) a filled contour plot will appear.

**Details**

The K-fold cross validation is performed in order to select the optimal value for  $\lambda$ , the penalty parameter in LASSO.

**Value**

The outcome is the same as in the R package `glmnet`. The extra addition is that if "graph = TRUE", then the plot of the cross-validated object is returned. The contains the logarithm of  $\lambda$  and the mean squared error. The numbers on top of the figure show the number of set of coefficients for each component, that are not zero.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

Friedman, J., Hastie, T. and Tibshirani, R. (2010) Regularization Paths for Generalized Linear Models via Coordinate Descent. Journal of Statistical Software, Vol. 33(1), 1-22.

**See Also**

[lasso.compreg](#), [lasso.klcompreg](#), [lassocoeff.plot](#), [cv.lasso.klcompreg](#), [comp.reg](#)

**Examples**

```
library(MASS)
y <- rdirich( 214, runif(4, 1, 3) )
x <- as.matrix( fgl[, 2:9] )
mod <- cv.lasso.compreg(y, x)
```

---

Cross-validation for the naive Bayes classifiers for compositional data

*Cross-validation for the naive Bayes classifiers for compositional data*

---

**Description**

Cross-validation for the naive Bayes classifiers for compositional data.

**Usage**

```
cv.compnb(x, ina, type = "beta", folds = NULL, n folds = 10,
          stratified = TRUE, seed = NULL, pred.ret = FALSE)
```

**Arguments**

x	A matrix with the available data, the predictor variables.
ina	A vector of data. The response variable, which is categorical (factor is acceptable).
type	The type of naive Bayes, "beta", "logitnorm", "cauchy", "laplace", "gamma", "normlog" or "weibull". For the last 4 distributions, the negative of the logarithm of the compositional data is applied first.
folds	A list with the indices of the folds.
n folds	The number of folds to be used. This is taken into consideration only if "folds" is NULL.

## 52 Cross-validation for the naive Bayes classifiers for compositional data using the alpha-transformation

stratified	Do you want the folds to be selected using stratified random sampling? This preserves the analogy of the samples of each group. Make this TRUE if you wish.
seed	You can specify your own seed number here or leave it NULL.
pred.ret	If you want the predicted values returned set this to TRUE.

### Value

A list including:

preds	If pred.ret is TRUE the predicted values for each fold are returned as elements in a list.
crit	A vector whose length is equal to the number of k and is the accuracy metric for each k. For the classification case it is the percentage of correct classification.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

### References

Friedman J., Hastie T. and Tibshirani R. (2017). The elements of statistical learning. New York: Springer.

### See Also

[comp.nb](#)

### Examples

```
x <- as.matrix(iris[, 1:4])
x <- x / rowSums(x)
mod <- cv.compnb(x, ina = iris[, 5] )
```

---

Cross-validation for the naive Bayes classifiers for compositional data using the alpha-transformation

*Cross-validation for the naive Bayes classifiers for compositional data using the  $\alpha$ -transformation*

---

### Description

Cross-validation for the naive Bayes classifiers for compositional data using the  $\alpha$ -transformation.

## Usage

```
alfanb.tune(x, ina, a = seq(-1, 1, by = 0.1), type = "gaussian",  
folds = NULL, n folds = 10, stratified = TRUE, seed = NULL)
```

## Arguments

x	A matrix with the available data, the predictor variables.
ina	A vector of data. The response variable, which is categorical (factor is acceptable).
a	The value of $\alpha$ for the $\alpha$ -transformation. This can be a vector of values or a single number.
type	The type of naive Bayes, "gaussian", "cauchy" or "laplace".
folds	A list with the indices of the folds.
n folds	The number of folds to be used. This is taken into consideration only if "folds" is NULL.
stratified	Do you want the folds to be selected using stratified random sampling? This preserves the analogy of the samples of each group. Make this TRUE if you wish.
seed	You can specify your own seed number here or leave it NULL.

## Details

This function estimates the performance of the naive Bayes classifier for each value of  $\alpha$  of the  $\alpha$ -transformation.

## Value

A list including:

crit	A vector whose length is equal to the number of k and is the accuracy metric for each k. For the classification case it is the percentage of correct classification.
------	--

## Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

## References

Friedman J., Hastie T. and Tibshirani R. (2017). The elements of statistical learning. New York: Springer.

## See Also

[alfa.nb](#), [alfarda.tune](#), [compknn.tune](#), [cv.dda](#), [cv.compnb](#)

**Examples**

```
x <- as.matrix(iris[, 1:4])
x <- x / rowSums(x)
mod <- alfanb.tune(x, ina = iris[, 5], a = c(0, 0.1, 0.2) )
```

---

Cross-validation for the SCLS model

*Cross-validation for the SCLS model*

---

**Description**

Cross-validation for the SCLS model.

**Usage**

```
cv.scls(y, x, nfolds = 10, folds = NULL, seed = NULL)
```

**Arguments**

<code>y</code>	A matrix with compositional response data. Zero values are allowed.
<code>x</code>	A matrix with compositional predictors. Zero values are allowed.
<code>nfolds</code>	The number of folds to be used. This is taken into consideration only if the folds argument is not supplied.
<code>folds</code>	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.
<code>seed</code>	You can specify your own seed number here or leave it NULL.

**Details**

The function performs k-fold cross-validation for the least squares regression where the beta coefficients are constrained to be positive and sum to 1.

**Value**

A list including:

<code>runtime</code>	The runtime of the cross-validation procedure.
<code>kl</code>	The Kullback-Leibler divergences for all runs.
<code>js</code>	The Jensen-Shannon divergences for all runs.
<code>perf</code>	The average Kullback-Leibler divergence and average Jensen-Shannon divergence.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

## References

Tsagris. M. (2024). Constrained least squares simplicial-simplicial regression. <https://arxiv.org/pdf/2403.19835.pdf>

## See Also

[scls](#), [cv.tflr](#), [klalfapcr.tune](#)

## Examples

```
library(MASS)
set.seed(1234)
y <- rdir(214, runif(3, 1, 3))
x <- as.matrix(fgl[, 2:9])
x <- x / rowSums(x)
mod <- cv.scls(y, x, nfolds = 5, seed = 12345)
mod
```

---

Cross-validation for the SCRQ model

*Cross-validation for the SCRQ model*

---

## Description

Cross-validation for the SCRQ model.

## Usage

```
cv.scrq(y, x, nfolds = 10, folds = NULL, seed = NULL)
```

## Arguments

<code>y</code>	A matrix with compositional response data. Zero values are allowed.
<code>x</code>	A matrix with compositional predictors. Zero values are allowed.
<code>nfolds</code>	The number of folds to be used. This is taken into consideration only if the folds argument is not supplied.
<code>folds</code>	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.
<code>seed</code>	You can specify your own seed number here or leave it NULL.

## Details

The function performs k-fold cross-validation for the absolute regression where the beta coefficients are constrained to be positive and sum to 1.

**Value**

A list including:

runtime	The runtime of the cross-validation procedure.
kl	The Kullback-Leibler divergences for all runs.
js	The Jensen-Shannon divergences for all runs.
perf	The average Kullback-Leibler divergence and average Jensen-Shannon divergence.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Tsagris, M. (2024). Constrained least squares simplicial-simplicial regression. <https://arxiv.org/pdf/2403.19835.pdf>

**See Also**

[scrq](#), [cv.scls](#), [cv.tflr](#)

**Examples**

```
library(MASS)
set.seed(1234)
y <- rdirichlet(214, runif(3, 1, 3))
x <- as.matrix(fgl[, 2:9])
x <- x / rowSums(x)
mod <- cv.scrq(y, x, nfolds = 5, seed = 12345)
mod
```

---

Density of compositional data from Gaussian mixture models

*Simulation of compositional data from Gaussian mixture models*

---

**Description**

Simulation of compositional data from Gaussian mixture models.

**Usage**

```
dmix.compnorm(x, mu, sigma, prob, type = "alr", logged = TRUE)
```



**Arguments**

<code>x</code>	A vector or a matrix with compositional data.
<code>prob</code>	A vector with mixing probabilities. Its length is equal to the number of clusters.
<code>mu</code>	A matrix where each row corresponds to the mean vector of each cluster.
<code>sigma</code>	An array consisting of the covariance matrix of each cluster.
<code>type</code>	The type of transformation used, either the additive log-ratio ("alr"), the isometric log-ratio ("ilr") or the pivot coordinate ("pivot") transformation.
<code>logged</code>	A boolean variable specifying whether the logarithm of the density values to be returned. It is set to TRUE by default.

**Details**

A sample from a multivariate Gaussian mixture model is generated.

**Value**

A vector with the density values.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Ryan P. Browne, Aisha ElSherbiny and Paul D. McNicholas (2015). R package mixture: Mixture Models for Clustering and Classification.

**See Also**

[mix.compnorm](#), [bic.mixcompnorm](#)

**Examples**

```
p <- c(1/3, 1/3, 1/3)
mu <- matrix(nrow = 3, ncol = 4)
s <- array( dim = c(4, 4, 3) )
x <- as.matrix(iris[, 1:4])
ina <- as.numeric(iris[, 5])
mu <- rowsum(x, ina) / 50
s[, , 1] <- cov(x[ina == 1, ])
s[, , 2] <- cov(x[ina == 2, ])
s[, , 3] <- cov(x[ina == 3, ])
y <- rmixcomp(100, p, mu, s, type = "alr")$x
mod <- dmix.compnorm(y, mu, s, p)
```

---

Density of the Flexible Dirichlet distribution

*Density of the Flexible Dirichlet distribution*

---

### Description

Density of the Flexible Dirichlet distribution

### Usage

```
dfd(x, alpha, prob, tau)
```

### Arguments

x	A vector or a matrix with compositional data.
alpha	A vector of the non-negative $\alpha$ parameters.
prob	A vector of the clusters' probabilities. It must sum to one.
tau	The non-negative scalar <i>tau</i> parameter.

### Details

For more information see the references and the package FlxeDir.

### Value

The density value(s).

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

### References

Ongaro A. and Migliorati S. (2013). A generalization of the Dirichlet distribution. *Journal of Multivariate Analysis*, 114, 412–426.

Migliorati S., Ongaro A. and Monti G. S. (2017). A structured Dirichlet mixture model for compositional data: inferential and applicative issues. *Statistics and Computing*, 27, 963–983.

### See Also

[rfd](#)

**Examples**

```
alpha <- c(12, 11, 10)
prob <- c(0.25, 0.25, 0.5)
tau <- 8
x <- rfd(20, alpha, prob, tau)
dfd(x, alpha, prob, tau)
```

---

Density of the folded normal distribution  
*Density of the folded model normal distribution*

---

**Description**

Density of the folded model normal distribution.

**Usage**

```
dfolded(x, a, p, mu, su, logged = TRUE)
```

**Arguments**

x	A vector or a matrix with compositional data. No zeros are allowed.
a	The value of $\alpha$ .
p	The probability inside the simplex of the folded model.
mu	The mean vector.
su	The covariance matrix.
logged	A boolean variable specifying whether the logarithm of the density values to be returned. It is set to TRUE by default.

**Details**

Density values of the folded model.

**Value**

The density value(s).

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Tsagris M. and Stewart C. (2020). A folded model for compositional data analysis. Australian and New Zealand Journal of Statistics, 62(2): 249-277. <https://arxiv.org/pdf/1802.07330.pdf>

**See Also**

[rfolded](#), [a.est](#), [folded.contour](#)

**Examples**

```
s <- c(0.1490676523, -0.4580818209, 0.0020395316, -0.0047446076, -0.4580818209,
1.5227259250, 0.0002596411, 0.0074836251, 0.0020395316, 0.0002596411,
0.0365384838, -0.0471448849, -0.0047446076, 0.0074836251, -0.0471448849,
0.0611442781)
s <- matrix(s, ncol = 4)
m <- c(1.715, 0.914, 0.115, 0.167)
x <- rfolded(100, m, s, 0.5)
mod <- a.est(x)
den <- dfolded(x, mod$best, mod$p, mod$mu, mod$su)
```

---

Density values of a Dirichlet distribution

*Density values of a Dirichlet distribution*

---

**Description**

Density values of a Dirichlet distribution.

**Usage**

```
ddiri(x, a, logged = TRUE)
```

**Arguments**

<code>x</code>	A matrix containing compositional data. This can be a vector or a matrix with the data.
<code>a</code>	A vector of parameters. Its length must be equal to the number of components, or columns of the matrix with the compositional data and all values must be greater than zero.
<code>logged</code>	A boolean variable specifying whether the logarithm of the density values to be returned. It is set to TRUE by default.

**Details**

The density of the Dirichlet distribution for a vector or a matrix of compositional data is returned.

**Value**

A vector with the density values.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Ng Kai Wang, Guo-Liang Tian and Man-Lai Tang (2011). Dirichlet and related distributions: Theory, methods and applications. John Wiley & Sons.

**See Also**

[dgendiri](#), [diri.nr](#), [diri.est](#), [diri.contour](#), [rdiri](#), [dda](#)

**Examples**

```
x <- rdiri( 100, c(5, 7, 4, 8, 10, 6, 4) )
a <- diri.est(x)
f <- ddiri(x, a$param)
sum(f)
a
```

---

Density values of a generalised Dirichlet distribution

*Density values of a generalised Dirichlet distribution*

---

**Description**

Density values of a generalised Dirichlet distribution.

**Usage**

```
dgendiri(x, a, b, logged = TRUE)
```

**Arguments**

x	A matrix containing compositional data. This can be a vector or a matrix with the data.
a	A numerical vector with the shape parameter values of the Gamma distribution.
b	A numerical vector with the scale parameter values of the Gamma distribution.
logged	A boolean variable specifying whether the logarithm of the density values to be returned. It is set to TRUE by default.

**Details**

The density of the Dirichlet distribution for a vector or a matrix of compositional data is returned.

**Value**

A vector with the density values.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Ng Kai Wang, Guo-Liang Tian and Man-Lai Tang (2011). Dirichlet and related distributions: Theory, methods and applications. John Wiley & Sons.

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

**See Also**

[ddiri](#), [rgendiri](#), [diri.est](#), [diri.contour](#), [rdiri](#), [dda](#)

**Examples**

```
a <- c(1, 2, 3)
b <- c(2, 3, 4)
x <- rgendiri(100, a, b)
y <- dgendiri(x, a, b)
```

---

Density values of a mixture of Dirichlet distributions

*Density values of a mixture of Dirichlet distributions*

---

**Description**

Density values of a mixture of Dirichlet distributions.

**Usage**

```
dmixdiri(x, a, prob, logged = TRUE)
```

**Arguments**

x	A vector or a matrix with compositional data. Zeros are not allowed.
a	A matrix where each row contains the parameters of each Dirichlet component.
prob	A vector with the mixing probabilities.
logged	A boolean variable specifying whether the logarithm of the density values to be returned. It is set to TRUE by default.

**Details**

The density of the mixture of Dirichlet distribution for a vector or a matrix of compositional data is returned.

**Value**

A vector with the density values.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Ye X., Yu Y. K. and Altschul S. F. (2011). On the inference of Dirichlet mixture priors for protein sequence comparison. *Journal of Computational Biology*, 18(8), 941-954.

**See Also**

[rmixdiri](#), [mixdiri.contour](#)

**Examples**

```
a <- matrix( c(12, 30, 45, 32, 50, 16), byrow = TRUE, ncol = 3)
prob <- c(0.5, 0.5)
x <- rmixdiri(100, a, prob)$x
f <- dmixdiri(x, a, prob)
```

---

Dirichlet discriminant analysis  
*Dirichlet discriminant analysis*

---

**Description**

Dirichlet discriminant analysis.

**Usage**

```
dda(xnew, x, ina)
```

**Arguments**

xnew	A matrix with the new compositional predictor data whose class you want to predict. Zeros are allowed.
x	A matrix with the available compositional predictor data. Zeros are allowed.
ina	A vector of data. The response variable, which is categorical (factor is acceptable).

**Details**

The function performs maximum likelihood discriminant analysis using the Dirichlet distribution.

**Value**

A vector with the estimated group.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Friedman J., Hastie T. and Tibshirani R. (2017). The elements of statistical learning. New York: Springer.

Thomas P. Minka (2003). Estimating a Dirichlet distribution. <http://research.microsoft.com/en-us/um/people/minka/papers/dirichlet/minka-dirichlet.pdf>

Ng Kai Wang, Guo-Liang Tian and Man-Lai Tang (2011). Dirichlet and related distributions: Theory, methods and applications. John Wiley & Sons.

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

**See Also**

[cv.dda](#), [comp.nb](#), [alfa.rda](#), [alfa.knn](#), [comp.knn](#), [mix.compnorm](#), [diri.reg](#), [zadr](#)

**Examples**

```
x <- Compositional::rdiri(100, runif(5) )
ina <- rbinom(100, 1, 0.5) + 1
mod <- dda(x, x, ina )
```

---

Dirichlet random values simulation

*Dirichlet random values simulation*

---

**Description**

Dirichlet random values simulation.

**Usage**

```
rdiri(n, a)
```



**Arguments**

n                    The sample size, a numerical value.  
a                    A numerical vector with the parameter values.

**Details**

The algorithm is straightforward, for each vector, independent gamma values are generated and then divided by their total sum.

**Value**

A matrix with the simulated data.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Giorgos Athineou <gioathineou@gmail.com>.

**References**

Ng Kai Wang, Guo-Liang Tian and Man-Lai Tang (2011). Dirichlet and related distributions: Theory, methods and applications. John Wiley & Sons.

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

**See Also**

[diri.est](#), [diri.nr](#), [diri.contour](#), [rgendiri](#)

**Examples**

```
x <- rdiri( 100, c(5, 7, 1, 3, 10, 2, 4) )  
diri.est(x)
```

---

Dirichlet regression    *Dirichlet regression*

---

**Description**

Dirichlet regression.

**Usage**

```
diri.reg(y, x, plot = FALSE, xnew = NULL)
```

```
diri.reg2(y, x, xnew = NULL)
```

```
diri.reg3(y, x, xnew = NULL)
```

**Arguments**

y	A matrix with the compositional data (dependent variable). Zero values are not allowed.
x	The predictor variable(s), they can be either continuous or categorical or both.
plot	A boolean variable specifying whether to plot the leverage values of the observations or not. This is taken into account only when xnew = NULL.
xnew	If you have new data use it, otherwise leave it NULL.

**Details**

A Dirichlet distribution is assumed for the regression. This involves numerical optimization. The function "diri.reg2()" allows for the covariates to be linked with the precision parameter  $\phi$  via the exponential link function  $\phi = e^{x*b}$ . The function "diri.reg3()" links the covariates to the alpha parameters of the Dirichlet distribution, i.e. it uses the classical parametrization of the distribution. This means, that there is a set of regression parameters for each component.

**Value**

A list including:

runtime	The time required by the regression.
loglik	The value of the log-likelihood.
phi	The precision parameter. If covariates are linked with it (function "diri.reg2()"), this will be a vector.
hipar	The coefficients of the phi parameter if it is linked to the covariates.
std.phi	The standard errors of the coefficients of the phi parameter if it is linked to the covariates.
log.phi	The logarithm of the precision parameter.
std.logphi	The standard error of the logarithm of the precision parameter.
be	The beta coefficients.
seb	The standard error of the beta coefficients.
sigma	The covariance matrix of the regression parameters (for the mean vector and the phi parameter)".
lev	The leverage values.
est	For the "diri.reg" this contains the fitted or the predicted values (if xnew is not NULL). For the "diri.reg2" if xnew is NULL, this is also NULL.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Giorgos Athineou <gioathineou@gmail.com>.

## References

Maier, Marco J. (2014) DirichletReg: Dirichlet Regression for Compositional Data in R. Research Report Series/Department of Statistics and Mathematics, 125. WU Vienna University of Economics and Business, Vienna. <http://epub.wu.ac.at/4077/1/Report125.pdf>

Gueorguieva, Ralitz, Robert Rosenheck, and Daniel Zelterman (2008). Dirichlet component regression and its applications to psychiatric data. *Computational statistics & data analysis* 52(12): 5344-5355.

Ng Kai Wang, Guo-Liang Tian and Man-Lai Tang (2011). Dirichlet and related distributions: Theory, methods and applications. John Wiley & Sons.

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

## See Also

[js.compreg](#), [kl.compreg](#), [ols.compreg](#), [comp.reg](#), [alfa.reg](#), [diri.nr](#), [dda](#)

## Examples

```
x <- as.vector(iris[, 4])
y <- as.matrix(iris[, 1:3])
y <- y / rowSums(y)
mod1 <- diri.reg(y, x)
mod2 <- diri.reg2(y, x)
mod3 <- comp.reg(y, x)
```

---

Distance based regression models for proportions

*Distance based regression models for proportions*

---

## Description

Distance based regression models for proportions.

## Usage

```
ols.prop.reg(y, x, cov = FALSE, tol = 1e-07, maxiters = 100)
helling.prop.reg(y, x, tol = 1e-07, maxiters = 100)
```

## Arguments

<code>y</code>	A numerical vector proportions. 0s and 1s are allowed.
<code>x</code>	A matrix or a data frame with the predictor variables.
<code>cov</code>	Should the covariance matrix be returned? TRUE or FALSE.
<code>tol</code>	The tolerance value to terminate the Newton-Raphson algorithm. This is set to $10^{-9}$ by default.
<code>maxiters</code>	The maximum number of iterations before the Newton-Raphson is terminated automatically.

**Details**

We are using the Newton-Raphson, but unlike R's built-in function "glm" we do no checks and no extra calculations, or whatever. Simply the model. The functions accept binary responses as well (0 or 1).

**Value**

A list including:

sse	The sum of squares of errors for the "ols.prop.reg" function.
be	The estimated regression coefficients.
seb	The standard error of the regression coefficients if "cov" is TRUE.
covb	The covariance matrix of the regression coefficients in "ols.prop.reg" if "cov" is TRUE.
H	The Hellinger distance between the true and the observed proportions in "helling.prop.reg".
iters	The number of iterations required by the Newton-Raphson.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Papke L. E. & Wooldridge J. (1996). Econometric methods for fractional response variables with an application to 401(K) plan participation rates. *Journal of Applied Econometrics*, 11(6): 619–632.

McCullagh, Peter, and John A. Nelder. *Generalized linear models*. CRC press, USA, 2nd edition, 1989.

**See Also**

[propreg](#), [beta.reg](#)

**Examples**

```
y <- rbeta(100, 1, 4)
x <- matrix(rnorm(100 * 2), ncol = 2)
a1 <- ols.prop.reg(y, x)
a2 <- helling.prop.reg(y, x)
```

---

 Divergence based regression for compositional data

*Divergence based regression for compositional data*


---

## Description

Regression for compositional data based on the Kullback-Leibler the Jensen-Shannon divergence and the symmetric Kullback-Leibler divergence.

## Usage

```
kl.compreg(y, x, con = TRUE, B = 1, ncores = 1, xnew = NULL, tol = 1e-07, maxiters = 50)
js.compreg(y, x, con = TRUE, B = 1, ncores = 1, xnew = NULL)
tv.compreg(y, x, con = TRUE, B = 1, ncores = 1, xnew = NULL)
symkl.compreg(y, x, con = TRUE, B = 1, ncores = 1, xnew = NULL)
hellinger.compreg(y, x, con = TRUE, B = 1, ncores = 1, xnew = NULL)
```

## Arguments

y	A matrix with the compositional data (dependent variable). Zero values are allowed.
x	The predictor variable(s), they can be either continuous or categorical or both.
con	If this is TRUE (default) then the constant term is estimated, otherwise the model includes no constant term.
B	If B is greater than 1 bootstrap estimates of the standard error are returned. If B=1, no standard errors are returned.
ncores	If ncores is 2 or more parallel computing is performed. This is to be used for the case of bootstrap. If B=1, this is not taken into consideration.
xnew	If you have new data use it, otherwise leave it NULL.
tol	The tolerance value to terminate the Newton-Raphson procedure.
maxiters	The maximum number of Newton-Raphson iterations.

## Details

In the `kl.compreg()` the Kullback-Leibler divergence is adopted as the objective function. In case of problematic convergence the "multinom" function by the "nnet" package is employed. This will obviously be slower. The `js.compreg()` uses the Jensen-Shannon divergence and the `symkl.compreg()` uses the symmetric Kullback-Leibler divergence. The `tv.compreg()` uses the Total Variation divergence. There is no actual log-likelihood for the last three regression models. The `hellinger.compreg()` minimizes the Hellinger distance.

**Value**

A list including:

<code>runtime</code>	The time required by the regression.
<code>iters</code>	The number of iterations required by the Newton-Raphson in the <code>kl.compreg</code> function.
<code>loglik</code>	The log-likelihood. This is actually a quasi multinomial regression. This is basically half the negative deviance, or $-\sum_{i=1}^n y_i \log y_i / \hat{y}_i$ .
<code>be</code>	The beta coefficients.
<code>covbe</code>	The covariance matrix of the beta coefficients, if bootstrap is chosen, i.e. if <code>B &gt; 1</code> .
<code>est</code>	The fitted values of <code>xnew</code> if <code>xnew</code> is not <code>NULL</code> .

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)> and Giorgos Athineou <[gioathineou@gmail.com](mailto:gioathineou@gmail.com)>.

**References**

Murteira Jose MR, and Joaquim JS Ramalho (2016). Regression analysis of multivariate fractional data. *Econometric Reviews* 35(4): 515-552.

Tsagris Michail (2015). A novel, divergence based, regression for compositional data. Proceedings of the 28th Panhellenic Statistics Conference, 15-18/4/2015, Athens, Greece. <https://arxiv.org/pdf/1511.07600.pdf>

Endres D. M. and Schindelin J. E. (2003). A new metric for probability distributions. *Information Theory, IEEE Transactions on* 49, 1858-1860.

Osterreicher F. and Vajda I. (2003). A new class of metric divergences on probability spaces and its applicability in statistics. *Annals of the Institute of Statistical Mathematics* 55, 639-653.

Alenazi A. A. (2022). f-divergence regression models for compositional data. *Pakistan Journal of Statistics and Operation Research*, 18(4): 867–882.

**See Also**

[diri.reg](#), [ols.compreg](#), [comp.reg](#)

**Examples**

```
library(MASS)
x <- as.vector(fgl[, 1])
y <- as.matrix(fgl[, 2:9])
y <- y / rowSums(y)
mod1<- kl.compreg(y, x, B = 1, ncores = 1)
mod2 <- js.compreg(y, x, B = 1, ncores = 1)
```

---

Divergence based regression for compositional data with compositional data in the covariates side using the alpha-transformation

*Divergence based regression for compositional data with compositional data in the covariates side using the  $\alpha$ -transformation*

---

## **Description**

Divergence based regression for compositional data with compositional data in the covariates side using the  $\alpha$ -transformation.

## **Usage**

```
kl.alfapcr(y, x, covar = NULL, a, k, xnew = NULL, B = 1, ncores = 1, tol = 1e-07, maxiters = 50)
```

## **Arguments**

y	A numerical matrix with compositional data with or without zeros.
x	A matrix with the predictor variables, the compositional data. Zero values are allowed.
covar	If you have other covariates as well put them here.
a	The value of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ the isometric log-ratio transformation is applied.
k	A number at least equal to 1. How many principal components to use.
xnew	A matrix containing the new compositional data whose response is to be predicted. If you have no new data, leave this NULL as is by default.
B	If B is greater than 1 bootstrap estimates of the standard error are returned. If B=1, no standard errors are returned.
ncores	If ncores is 2 or more parallel computing is performed. This is to be used for the case of bootstrap. If B=1, this is not taken into consideration.
tol	The tolerance value to terminate the Newton-Raphson procedure.
maxiters	The maximum number of Newton-Raphson iterations.

## **Details**

The  $\alpha$ -transformation is applied to the compositional data first, the first k principal component scores are calculated and used as predictor variables for the Kullback-Leibler divergence based regression model.

## Value

A list including:

<code>runtime</code>	The time required by the regression.
<code>iters</code>	The number of iterations required by the Newton-Raphson in the <code>kl.compreg</code> function.
<code>loglik</code>	The log-likelihood. This is actually a quasi multinomial regression. This is basically minus the half deviance, or $-\sum_{i=1}^n y_i \log y_i / \hat{y}_i$ .
<code>be</code>	The beta coefficients.
<code>seb</code>	The standard error of the beta coefficients, if bootstrap is chosen, i.e. if <code>B &gt; 1</code> .
<code>est</code>	The fitted values of <code>xnew</code> if <code>xnew</code> is not <code>NULL</code> .

## Author(s)

Initial code by Abdulaziz Alenazi. Modifications by Michail Tsagris.

R implementation and documentation: Abdulaziz Alenazi <a.alenazi@nbu.edu.sa> and Michail Tsagris <mtsagris@uoc.gr>.

## References

- Alenazi A. (2019). Regression for compositional data with compositional data as predictor variables with or without zero values. *Journal of Data Science*, 17(1): 219-238. <https://jds-online.org/journal/JDS/article/136/file/pdf>
- Tsagris M. (2015). Regression analysis with compositional data containing zero values. *Chilean Journal of Statistics*, 6(2): 47-57. <http://arxiv.org/pdf/1508.01913v1.pdf>
- Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In *Proceedings of the 4th Compositional Data Analysis Workshop*, Girona, Spain. <http://arxiv.org/pdf/1106.1451.pdf>

## See Also

[klalfapcr.tune](#), [tflr](#), [glm.pcr](#), [alfapcr.tune](#)

## Examples

```
library(MASS)
y <- rdirichlet(214, runif(4, 1, 3))
x <- as.matrix(fgl[, 2:9])
x <- x / rowSums(x)
mod <- alfa.pcr(y = y, x = x, a = 0.7, k = 1)
mod
```



---

Divergence matrix of compositional data  
*Divergence matrix of compositional data*

---

**Description**

Divergence matrix of compositional data.

**Usage**

```
divergence(x, type = "kullback_leibler", vector = FALSE)
```

**Arguments**

x	A matrix with the compositional data.
type	This is either "kullback_leibler" (Kullback-Leibler, which computes the symmetric Kullback-Leibler divergence) or "jensen_shannon" (Jensen-Shannon) divergence.
vector	For return a vector instead a matrix.

**Details**

The function produces the distance matrix either using the Kullback-Leibler (distance) or the Jensen-Shannon (metric) divergence. The Kullback-Leibler refers to the symmetric Kullback-Leibler divergence.

**Value**

if the vector argument is FALSE a symmetric matrix with the divergences, otherwise a vector with the divergences.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Endres, D. M. and Schindelin, J. E. (2003). A new metric for probability distributions. Information Theory, IEEE Transactions on 49, 1858-1860.

Osterreicher, F. and Vajda, I. (2003). A new class of metric divergences on probability spaces and its applicability in statistics. Annals of the Institute of Statistical Mathematics 55, 639-653.

**See Also**

[comp.knn](#), [js.compreg](#)

**Examples**

```
x <- as.matrix(iris[1:20, 1:4])
x <- x / rowSums(x)
divergence(x)
```

---

Empirical likelihood hypothesis testing for two mean vectors

*Empirical likelihood hypothesis testing for two mean vectors*

---

**Description**

Empirical likelihood hypothesis testing for two mean vectors.

**Usage**

```
el.test2(y1, y2, R = 0, ncores = 1, graph = FALSE)
```

**Arguments**

y1	A matrix containing the Euclidean data of the first group.
y2	A matrix containing the Euclidean data of the second group.
R	If R is 0, the classical chi-square distribution is used, if R = 1, the corrected chi-square distribution (James, 1954) is used and if R = 2, the modified F distribution (Krishnamoorthy and Yanping, 2006) is used. If R is greater than 3 bootstrap calibration is performed.
ncores	How many to cores to use.
graph	A boolean variable which is taken into consideration only when bootstrap calibration is performed. IF TRUE the histogram of the bootstrap test statistic values is plotted.

**Details**

The  $H_0$  is that  $\boldsymbol{\mu}_1 = \boldsymbol{\mu}_2$  and the two constraints imposed by EL are

$$\frac{1}{n_j} \sum_{i=1}^{n_j} \left\{ [1 + \boldsymbol{\lambda}_j^T (\mathbf{x}_{ji} - \boldsymbol{\mu})]^{-1} (\mathbf{x}_{ji} - \boldsymbol{\mu}) \right\} = \mathbf{0},$$

where  $j = 1, 2$  and the  $\boldsymbol{\lambda}_j$ s are Lagrangian parameters introduced to maximize the above expression. Note that the maximization of is with respect to the  $\boldsymbol{\lambda}_j$ s. The probabilities of the  $j$ -th sample have the following form

$$p_{ji} = \frac{1}{n_j} [1 + \boldsymbol{\lambda}_j^T (\mathbf{x}_{ji} - \boldsymbol{\mu})]^{-1}$$

. The log-likelihood ratio test statistic can be written as

$$\Lambda = \sum_{j=1}^2 \sum_{i=1}^{n_j} \log n_j p_{ij}.$$

The test is implemented by searching for the mean vector that minimizes the sum of the two one sample EL test statistics.

**Value**

A list including:

<code>test</code>	The empirical likelihood test statistic value.
<code>modif.test</code>	The modified test statistic, either via the chi-square or the F distribution.
<code>dof</code>	Three degrees of freedom of the chi-square or the F distribution.
<code>pvalue</code>	The asymptotic or the bootstrap p-value.
<code>mu</code>	The estimated common mean vector.
<code>runtime</code>	The runtime of the bootstrap calibration.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

**References**

- Amaral G.J.A., Dryden I.L. and Wood A.T.A. (2007). Pivotal bootstrap methods for k-sample problems in directional statistics and shape analysis. *Journal of the American Statistical Association*, 102(478): 695–707.
- Owen A. B. (2001). *Empirical likelihood*. Chapman and Hall/CRC Press.
- Owen A.B. (1988). Empirical likelihood ratio confidence intervals for a single functional. *Biometrika*, 75(2): 237–249.
- Preston S.P. and Wood A.T.A. (2010). Two-Sample Bootstrap Hypothesis Tests for Three-Dimensional Labelled Landmark Data. *Scandinavian Journal of Statistics*, 37(4): 568–587.

**See Also**

[eel.test2](#), [maovjames](#), [hotel2T2](#), [james](#)

**Examples**

```
e1.test2( y1 = as.matrix(iris[1:25, 1:4]), y2 = as.matrix(iris[26:50, 1:4]), R = 0 )
e1.test2( y1 = as.matrix(iris[1:25, 1:4]), y2 = as.matrix(iris[26:50, 1:4]), R = 1 )
e1.test2( y1 =as.matrix(iris[1:25, 1:4]), y2 = as.matrix(iris[26:50, 1:4]), R = 2 )
```

---

Energy test of equality of distributions using the alpha-transformation

*Energy test of equality of distributions using the  $\alpha$ -transformation*

---

### Description

Energy test of equality of distributions using the  $\alpha$ -transformation.

### Usage

```
aeqdist.etest(x, sizes, a = 1, R = 999)
```

### Arguments

x	A matrix with the compositional data with all groups stacked one under the other.
sizes	A numeric vector matrix with the sample sizes.
a	The value of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ the isometric log-ratio transformation is applied. If more than one values are supplied the energy distance of equality of distributions is applied for each value of $\alpha$ .
R	The number of permutations to apply in order to compute the approximate p-value.

### Details

The  $\alpha$ -transformation is applied to each composition and then the energy distance of equality of distributions is applied for each value of  $\alpha$  or for the single value of  $\alpha$ .

### Value

A numerical value or a numerical vector, depending on the length of the values of  $\alpha$ , with the approximate p-value(s) of the energy test.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

### References

Szekely, G. J. and Rizzo, M. L. (2004) Testing for Equal Distributions in High Dimension. InterStat, November (5).

Szekely, G. J. (2000) Technical Report 03-05: E-statistics: Energy of Statistical Samples. Department of Mathematics and Statistics, Bowling Green State University.

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain. <https://arxiv.org/pdf/1106.1451.pdf>

### See Also

[acor](#), [acor.tune](#), [alfa](#), [alfa.profile](#)

### Examples

```
y <- rdiri(50, c(3, 4, 5) )
x <- rdiri(60, c(3, 4, 5) )
aeqdist.etest( rbind(x, y), c(dim(x)[1], dim(y)[1]), a = c(-1, 0, 1) )
```

---

Estimating location and scatter parameters for compositional data

*Estimating location and scatter parameters for compositional data*

---

### Description

Estimating location and scatter parameters for compositional data in a robust and non robust way.

### Usage

```
comp.den(x, type = "alr", dist = "normal", tol = 1e-07)
```

### Arguments

x	A matrix containing compositional data. No zero values are allowed.
type	A boolean variable indicating the transformation to be used. Either "alr" or "ilr" corresponding to the additive or the isometric log-ratio transformation respectively.
dist	Takes values "normal", "t", "skewnorm", "rob" and "spatial". The first three options correspond to the parameters of the normal, t and skew normal distribution respectively. If it set to "rob" the MCD estimates are computed and if set to "spatial" the spatial median and spatial sign covariance matrix are computed.
tol	A tolerance level to terminate the process of finding the spatial median when dist = "spatial". This is set to 1e-09 by default.

### Details

This function calculates robust and non robust estimates of location and scatter.

### Value

A list including: The mean vector and covariance matrix mainly. Other parameters are also returned depending on the value of the argument "dist".

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

P. J. Rousseeuw and K. van Driessen (1999) A fast algorithm for the minimum covariance determinant estimator. *Technometrics* 41, 212-223.

Mardia K.V., Kent J.T., and Bibby J.M. (1979). *Multivariate analysis*. Academic press.

Aitchison J. (1986). *The statistical analysis of compositional data*. Chapman & Hall.

T. Karkkainen and S. Ayramo (2005). On computation of spatial median for robust data mining. *Evolutionary and Deterministic Methods for Design, Optimization and Control with Applications to Industrial and Societal Problems EUROGEN 2005*.

A Durre, D Vogel, DE Tyler (2014). The spatial sign covariance matrix with unknown location. *Journal of Multivariate Analysis*, 130: 107-117.

J. T. Kent, D. E. Tyler and Y. Vardi (1994) A curious likelihood identity for the multivariate t-distribution. *Communications in Statistics-Simulation and Computation* 23, 441-453.

Azzalini A. and Dalla Valle A. (1996). The multivariate skew-normal distribution. *Biometrika* 83(4): 715-726.

**See Also**

[spatmed.reg](#), [multivt](#)

**Examples**

```
library(MASS)
x <- as.matrix(iris[, 1:4])
x <- x / rowSums(x)
comp.den(x)
comp.den(x, type = "alr", dist = "t")
comp.den(x, type = "alr", dist = "spatial")
```

---

Estimation of the probability left outside the simplex when using the alpha-transformation

*Estimation of the probability left outside the simplex when using the alpha-transformation*

---

**Description**

Estimation of the probability left outside the simplex when using the alpha-transformationn.

**Usage**

```
probout(mu, su, a)
```

**Arguments**

mu	The mean vector.
su	The covariance matrix.
a	The value of $\alpha$ .

**Details**

When applying the  $\alpha$ -transformation based on a multivariate normal there might be probability left outside the simplex as the space of this transformation is a subspace of the Euclidean space. The function estimates the missing probability via Monte Carlo simulation using 40 million generated vectors.

**Value**

The estimated probability left outside the simplex.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

**References**

Tsagris M. and Stewart C. (2020). A folded model for compositional data analysis. Australian and New Zealand Journal of Statistics, 62(2): 249-277. <https://arxiv.org/pdf/1802.07330.pdf>

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain. <https://arxiv.org/pdf/1106.1451.pdf>

**See Also**

[alfa](#), [alpha.mle](#), [a.est](#), [rfolded](#)

**Examples**

```
s <- c(0.1490676523, -0.4580818209, 0.0020395316, -0.0047446076, -0.4580818209,
1.5227259250, 0.0002596411, 0.0074836251, 0.0020395316, 0.0002596411,
0.0365384838, -0.0471448849, -0.0047446076, 0.0074836251, -0.0471448849,
0.0611442781)
s <- matrix(s, ncol = 4)
m <- c(1.715, 0.914, 0.115, 0.167)
probout(m, s, 0.5)
```

---

Estimation of the value of alpha in the folded model

*Estimation of the value of  $\alpha$  in the folded model*

---

### Description

Estimation of the value of  $\alpha$  in the folded model.

### Usage

```
a.est(x)
```

### Arguments

x                    A matrix with the compositional data. No zero values are allowed.

### Details

This is a function for choosing or estimating the value of  $\alpha$  in the folded model (Tsagris and Stewart, 2020).

### Value

A list including:

runtime	The runtime of the algorithm.
best	The estimated optimal $\alpha$ of the folded model.
loglik	The maximised log-likelihood of the folded model.
p	The estimated probability inside the simplex of the folded model.
mu	The estimated mean vector of the folded model.
su	The estimated covariance matrix of the folded model.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

### References

- Tsagris M. and Stewart C. (2022). A Review of Flexible Transformations for Modeling Compositional Data. In *Advances and Innovations in Statistics and Data Science*, pp. 225–234. [https://link.springer.com/chapter/10.1007/978-3-031-08329-7\\_10](https://link.springer.com/chapter/10.1007/978-3-031-08329-7_10)
- Tsagris M. and Stewart C. (2020). A folded model for compositional data analysis. *Australian and New Zealand Journal of Statistics*, 62(2): 249-277. <https://arxiv.org/pdf/1802.07330.pdf>
- Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In *Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain*. <https://arxiv.org/pdf/1106.1451.pdf>



**See Also**

[alfa.profile](#), [alfa](#), [alfainv](#), [alpha.mle](#)

**Examples**

```
x <- as.matrix(iris[, 1:4])
x <- x / rowSums(x)
alfa.tune(x)
a.est(x)
```

---

Estimation of the value of alpha via the profile log-likelihood

*Estimation of the value of  $\alpha$  via the alfa profile log-likelihood*

---

**Description**

Estimation of the value of  $\alpha$  via the alfa profile log-likelihood.

**Usage**

```
alfa.profile(x, a = seq(-1, 1, by = 0.01))
```

**Arguments**

x	A matrix with the compositional data. Zero values are not allowed.
a	A grid of values of $\alpha$ .

**Details**

For every value of  $\alpha$  the normal likelihood (see the refernece) is computed. At the end, the plot of the values is constructed.

**Value**

A list including:

res	The chosen value of $\alpha$ , the corresponding log-likelihood value and the log-likelihood when $\alpha = 0$ .
ci	An asymptotic 95% confidence interval computed from the log-likelihood ratio test.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Giorgos Athineou <gioathineou@gmail.com>.

**References**

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain. <https://arxiv.org/pdf/1106.1451.pdf>

**See Also**

[alfa.tune](#), [alfa](#), [alfainv](#)

**Examples**

```
x <- as.matrix(iris[, 1:4])
x <- x / rowSums(x)
alfa.tune(x)
alfa.profile(x)
```

---

Exponential empirical likelihood hypothesis testing for two mean vectors

*Exponential empirical likelihood hypothesis testing for two mean vectors*

---

**Description**

Exponential empirical likelihood hypothesis testing for two mean vectors.

**Usage**

```
ee1.test2(y1, y2, tol = 1e-07, R = 0, graph = FALSE)
```

**Arguments**

<code>y1</code>	A matrix containing the Euclidean data of the first group.
<code>y2</code>	A matrix containing the Euclidean data of the second group.
<code>tol</code>	The tolerance level used to terminate the Newton-Raphson algorithm.
<code>R</code>	If <code>R</code> is 0, the classical chi-square distribution is used, if <code>R</code> = 1, the corrected chi-square distribution (James, 1954) is used and if <code>R</code> = 2, the modified F distribution (Krishnamoorthy and Yanping, 2006) is used. If <code>R</code> is greater than 3 bootstrap calibration is performed.
<code>graph</code>	A boolean variable which is taken into consideration only when bootstrap calibration is performed. IF TRUE the histogram of the bootstrap test statistic values is plotted.

### Details

Exponential empirical likelihood or exponential tilting was first introduced by Efron (1981) as a way to perform a "tilted" version of the bootstrap for the one sample mean hypothesis testing. Similarly to the empirical likelihood, positive weights  $p_i$ , which sum to one, are allocated to the observations, such that the weighted sample mean  $\bar{\mathbf{x}}$  is equal to some population mean  $\boldsymbol{\mu}$ , under the  $H_0$ . Under  $H_1$  the weights are equal to  $\frac{1}{n}$ , where  $n$  is the sample size. Following Efron (1981), the choice of  $p_i$ s will minimize the Kullback-Leibler distance from  $H_0$  to  $H_1$

$$D(L_0, L_1) = \sum_{i=1}^n p_i \log(np_i),$$

subject to the constraint  $\sum_{i=1}^n p_i \mathbf{x}_i = \boldsymbol{\mu}$ . The probabilities take the form

$$p_i = \frac{e^{\boldsymbol{\lambda}^T \mathbf{x}_i}}{\sum_{j=1}^n e^{\boldsymbol{\lambda}^T \mathbf{x}_j}}$$

and the constraint becomes

$$\frac{\sum_{i=1}^n e^{\boldsymbol{\lambda}^T \mathbf{x}_i} (\mathbf{x}_i - \boldsymbol{\mu})}{\sum_{j=1}^n e^{\boldsymbol{\lambda}^T \mathbf{x}_j}} = 0 \Rightarrow \frac{\sum_{i=1}^n \mathbf{x}_i e^{\boldsymbol{\lambda}^T \mathbf{x}_i}}{\sum_{j=1}^n e^{\boldsymbol{\lambda}^T \mathbf{x}_j}} - \boldsymbol{\mu} = 0.$$

Similarly to empirical likelihood a numerical search over  $\boldsymbol{\lambda}$  is required.

We can derive the asymptotic form of the test statistic in the two sample means case but in a simpler form, generalizing the approach of Jing and Robinson (1997) to the multivariate case as follows. The three constraints are

$$\begin{aligned} \left( \sum_{j=1}^{n_1} e^{\boldsymbol{\lambda}_1^T \mathbf{x}_j} \right)^{-1} \left( \sum_{i=1}^{n_1} \mathbf{x}_i e^{\boldsymbol{\lambda}_1^T \mathbf{x}_i} \right) - \boldsymbol{\mu} &= \mathbf{0} \\ \left( \sum_{j=1}^{n_2} e^{\boldsymbol{\lambda}_2^T \mathbf{y}_j} \right)^{-1} \left( \sum_{i=1}^{n_2} \mathbf{y}_i e^{\boldsymbol{\lambda}_2^T \mathbf{y}_i} \right) - \boldsymbol{\mu} &= \mathbf{0} \\ n_1 \boldsymbol{\lambda}_1 + n_2 \boldsymbol{\lambda}_2 &= \mathbf{0}. \end{aligned}$$

Similarly to EL the sum of a linear combination of the  $\boldsymbol{\lambda}$ s is set to zero. We can equate the first two constraints of

$$\left( \sum_{j=1}^{n_1} e^{\boldsymbol{\lambda}_1^T \mathbf{x}_j} \right)^{-1} \left( \sum_{i=1}^{n_1} \mathbf{x}_i e^{\boldsymbol{\lambda}_1^T \mathbf{x}_i} \right) = \left( \sum_{j=1}^{n_2} e^{\boldsymbol{\lambda}_2^T \mathbf{y}_j} \right)^{-1} \left( \sum_{i=1}^{n_2} \mathbf{y}_i e^{\boldsymbol{\lambda}_2^T \mathbf{y}_i} \right).$$

Also, we can write the third constraint of as  $\boldsymbol{\lambda}_2 = -\frac{n_1}{n_2} \boldsymbol{\lambda}_1$  and thus rewrite the first two constraints as

$$\left( \sum_{j=1}^{n_1} e^{\boldsymbol{\lambda}_1^T \mathbf{x}_j} \right)^{-1} \left( \sum_{i=1}^{n_1} \mathbf{x}_i e^{\boldsymbol{\lambda}_1^T \mathbf{x}_i} \right) = \left( \sum_{j=1}^{n_2} e^{-\frac{n_1}{n_2} \boldsymbol{\lambda}_1^T \mathbf{y}_j} \right)^{-1} \left( \sum_{i=1}^{n_2} \mathbf{y}_i e^{-\frac{n_1}{n_2} \boldsymbol{\lambda}_1^T \mathbf{y}_i} \right).$$

This trick allows us to avoid the estimation of the common mean. It is not possible though to do this in the empirical likelihood method. Instead of minimisation of the sum of the one-sample test statistics from the common mean, we can define the probabilities by searching for the  $\boldsymbol{\lambda}$  which makes the last equation hold true. The third constraint of is a convenient constraint, but Jing and Robinson (1997) mention that even though as a constraint is simple it does not lead to second-order accurate confidence intervals unless the two sample sizes are equal. Asymptotically, the test statistic follows a  $\chi_d^2$  under the null hypothesis.

**Value**

A list including:

<code>test</code>	The empirical likelihood test statistic value.
<code>modif.test</code>	The modified test statistic, either via the chi-square or the F distribution.
<code>dof</code>	The degrees of freedom of the chi-square or the F distribution.
<code>pvalue</code>	The asymptotic or the bootstrap p-value.
<code>mu</code>	The estimated common mean vector.
<code>runtime</code>	The runtime of the bootstrap calibration.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

**References**

- Efron B. (1981) Nonparametric standard errors and confidence intervals. *Canadian Journal of Statistics*, 9(2): 139–158.
- Jing B.Y. and Wood A.T.A. (1996). Exponential empirical likelihood is not Bartlett correctable. *Annals of Statistics*, 24(1): 365–369.
- Jing B.Y. and Robinson J. (1997). Two-sample nonparametric tilting method. *Australian Journal of Statistics*, 39(1): 25–34.
- Owen A.B. (2001). *Empirical likelihood*. Chapman and Hall/CRC Press.
- Preston S.P. and Wood A.T.A. (2010). Two-Sample Bootstrap Hypothesis Tests for Three-Dimensional Labelled Landmark Data. *Scandinavian Journal of Statistics* 37(4): 568–587.
- Tsagris M., Preston S. and Wood A.T.A. (2017). Nonparametric hypothesis testing for equality of means on the simplex. *Journal of Statistical Computation and Simulation*, 87(2): 406–422.

**See Also**

[el.test2](#), [maovjames](#), [hotel2T2](#), [james](#)

**Examples**

```
y1 = as.matrix(iris[1:25, 1:4])
y2 = as.matrix(iris[26:50, 1:4])
eel.test2(y1, y2)
eel.test2(y1, y2 )
eel.test2( y1, y2 )
```

---

Fast estimation of the value of alpha  
*Fast estimation of the value of  $\alpha$*

---

## Description

Fast estimation of the value of  $\alpha$ .

## Usage

```
alfa.tune(x, B = 1, ncores = 1)
```

## Arguments

x	A matrix with the compositional data. No zero values are allowed.
B	If no (bootstrap based) confidence intervals should be returned this should be 1 and more than 1 otherwise.
ncores	If ncores is greater than 1 parallel computing is performed. It is advisable to use it if you have many observations and or many variables, otherwise it will slow down the process.

## Details

This is a faster function than [alfa.profile](#) for choosing the value of  $\alpha$ .

## Value

A vector with the best alpha, the maximised log-likelihood and the log-likelihood at  $\alpha = 0$ , when  $B = 1$  (no bootstrap). If  $B > 1$  a list including:

param	The best alpha and the value of the log-likelihood, along with the 95% bootstrap based confidence intervals.
message	A message with some information about the histogram.
runtime	The time (in seconds) of the process.

## Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)> and Giorgos Athineou <[gioathineou@gmail.com](mailto:gioathineou@gmail.com)>.

## References

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain. <https://arxiv.org/pdf/1106.1451.pdf>

**See Also**

[alfa.profile](#), [alfa](#), [alfainv](#)

**Examples**

```
library(MASS)
x <- as.matrix(iris[, 1:4])
x <- x / rowSums(x)
alfa.tune(x)
alfa.profile(x)
```

---

Gaussian mixture models for compositional data

*Gaussian mixture models for compositional data*

---

**Description**

Gaussian mixture models for compositional data.

**Usage**

```
mix.compnorm(x, g, model, type = "alr", veo = FALSE)
```

**Arguments**

- |       |   |
|-------|---|
| x     | A matrix with the compositional data.   |
| g     | How many clusters to create.  |
| model | The type of model to be used. <ol style="list-style-type: none"> <li>1. "EII": All groups have the same diagonal covariance matrix, with the same variance for all variables.</li> <li>2. "VII": Different diagonal covariance matrices, with the same variance for all variables within each group.</li> <li>3. "EEI": All groups have the same diagonal covariance matrix.</li> <li>4. "VEI": Different diagonal covariance matrices. If we make all covariance matrices have determinant 1, (divide the matrix with the <math>p</math>-th root of its determinant) then all covariance matrices will be the same.</li> <li>5. "EVI": Different diagonal covariance matrices with the same determinant.</li> <li>6. "VVI": Different diagonal covariance matrices, with nothing in common.</li> <li>7. "EEE": All covariance matrices are the same.</li> <li>8. "EEV": Different covariance matrices, but with the same determinant and in addition, if we make them have determinant 1, they will have the same trace.</li> <li>9. "VEV": Different covariance matrices but if we make the matrices have determinant 1, then they will have the same trace.</li> <li>10. "VVV": Different covariance matrices with nothing in common.</li> </ol> |

11. "EVE": Different covariance matrices, but with the same determinant. In addition, calculate the eigenvectors for each covariance matrix and you will see the extra similarities.
  12. "VVE": Different covariance matrices, but they have something in common with their directions. Calculate the eigenvectors of each covariance matrix and you will see the similarities.
  13. "VEE": Different covariance matrices, but if we make the matrices have determinant 1, then they will have the same trace. In addition, calculate the eigenvectors for each covariance matrix and you will see the extra similarities.
  14. "EVV": Different covariance matrices, but with the same determinant.
- type      The type of transformation to be used, either the additive log-ratio ("alr"), the isometric log-ratio ("ilr") or the pivot coordinate ("pivot") transformation.
- veo        Stands for "Variables exceed observations". If TRUE then if the number variables in the model exceeds the number of observations, but the model is still fitted.

### Details

A log-ratio transformation is applied and then a Gaussian mixture model is constructed.

### Value

A list including:

- mu        A matrix where each row corresponds to the mean vector of each cluster.
- su        An array containing the covariance matrix of each cluster.
- prob     The estimated mixing probabilities.
- est       The estimated cluster membership values.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

### References

Ryan P. Browne, Aisha ElSherbiny and Paul D. McNicholas (2015). R package mixture: Mixture Models for Clustering and Classification.

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

### See Also

[bic.mixcompnorm](#), [rmixcomp](#), [mix.compnorm.contour](#), [alfa.mix.norm](#), [alfa.knn](#), [alfa.rda](#), [comp.nb](#)

**Examples**

```
x <- as.matrix(iris[, 1:4])
x <- x/ rowSums(x)
mod1 <- mix.compnorm(x, 3, model = "EII" )
mod2 <- mix.compnorm(x, 4, model = "VII")
```

---

Gaussian mixture models for compositional data using the alpha-transformation

*Gaussian mixture models for compositional data using the  $\alpha$ -transformation*

---

**Description**

Gaussian mixture models for compositional data using the  $\alpha$ -transformation.

**Usage**

```
alfa.mix.norm(x, g, a, model, veo = FALSE)
```

**Arguments**

- |       |  |
|-------|--|
| x     | A matrix with the compositional data.  |
| g     | How many clusters to create.   |
| a     | The value of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ the isometric log-ratio transformation is applied.   |
| model | The type of model to be used. <ol style="list-style-type: none"> <li>"EII": All groups have the same diagonal covariance matrix, with the same variance for all variables.</li> <li>"VII": Different diagonal covariance matrices, with the same variance for all variables within each group.</li> <li>"EEI": All groups have the same diagonal covariance matrix.</li> <li>"VEI": Different diagonal covariance matrices. If we make all covariance matrices have determinant 1, (divide the matrix with the <math>p</math>-th root of its determinant) then all covariance matrices will be the same.</li> <li>"EVI": Different diagonal covariance matrices with the same determinant.</li> <li>"VVI": Different diagonal covariance matrices, with nothing in common.</li> <li>"EEE": All covariance matrices are the same.</li> <li>"EEV": Different covariance matrices, but with the same determinant and in addition, if we make them have determinant 1, they will have the same trace.</li> <li>"VEV": Different covariance matrices but if we make the matrices have determinant 1, then they will have the same trace.</li> </ol> |



10. "VVV": Different covariance matrices with nothing in common.
  11. "EVE": Different covariance matrices, but with the same determinant. In addition, calculate the eigenvectors for each covariance matrix and you will see the extra similarities.
  12. "VVE": Different covariance matrices, but they have something in common with their directions. Calculate the eigenvectors of each covariance matrix and you will see the similarities.
  13. "VEE": Different covariance matrices, but if we make the matrices have determinant 1, then they will have the same trace. In addition, calculate the eigenvectors for each covariance matrix and you will see the extra similarities.
  14. "EVV": Different covariance matrices, but with the same determinant.
- veo Stands for "Variables exceed observations". If TRUE then if the number variables in the model exceeds the number of observations, but the model is still fitted.

### Details

A log-ratio transformation is applied and then a Gaussian mixture model is constructed.

### Value

A list including:

- |      |   |
|------|---|
| mu   | A matrix where each row corresponds to the mean vector of each cluster. |
| su   | An array containing the covariance matrix of each cluster.              |
| prob | The estimated mixing probabilities.                                     |
| est  | The estimated cluster membership values.                                |

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

### References

Ryan P. Browne, Aisha ElSherbiny and Paul D. McNicholas (2015). R package mixture: Mixture Models for Clustering and Classification.

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain. <https://arxiv.org/pdf/1106.1451.pdf>

### See Also

[bic.alfamixnorm](#), [bic.mixcompnorm](#), [rmixcomp](#), [mix.compnorm.contour](#), [mix.compnorm](#), [alfa](#), [alfa.knn](#), [alfa.rda](#), [comp.nb](#)

**Examples**

```
x <- as.matrix(iris[, 1:4])
x <- x/ rowSums(x)
mod1 <- alfa.mix.norm(x, 3, 0.4, model = "EII" )
mod2 <- alfa.mix.norm(x, 4, 0.7, model = "VII")
```

---

Generalised Dirichlet random values simulation

*Generalised Dirichlet random values simulation*

---

**Description**

Generalised Dirichlet random values simulation.

**Usage**

```
rgendiri(n, a, b)
```

**Arguments**

n	The sample size, a numerical value.
a	A numerical vector with the shape parameter values of the Gamma distribution.
b	A numerical vector with the scale parameter values of the Gamma distribution.

**Details**

The algorithm is straightforward, for each vector, independent gamma values are generated and then divided by their total sum. The difference with `rdiri` is that here the Gamma distributed variables are not equally scaled.

**Value**

A matrix with the simulated data.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Ng Kai Wang, Guo-Liang Tian and Man-Lai Tang (2011). Dirichlet and related distributions: Theory, methods and applications. John Wiley & Sons.

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

**See Also**

[rdiri](#), [diri.est](#), [diri.nr](#), [diri.contour](#)

**Examples**

```
a <- c(1, 2, 3)
b <- c(2, 3, 4)
x <- rgendiri(100, a, b)
```

---

Generate random folds for cross-validation

*Generate random folds for cross-validation*

---

**Description**

Random folds for use in a cross validation are generated. There is the option for stratified splitting as well.

**Usage**

```
makefolds(ina, nfolds = 10, stratified = TRUE, seed = NULL)
```

**Arguments**

<code>ina</code>	A variable indicating the groupings.
<code>nfolds</code>	The number of folds to produce.
<code>stratified</code>	A boolean variable specifying whether stratified random (TRUE) or simple random (FALSE) sampling is to be used when producing the folds.
<code>seed</code>	You can specify your own seed number here or leave it NULL.

**Details**

I was inspired by the command in the package **TunePareto** in order to do the stratified version.

**Value**

A list with `nfolds` elements where each element is a fold containing the indices of the data.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

**See Also**

[compknn.tune](#)

**Examples**

```
a <- makefolds(iris[, 5], nfolds = 5, stratified = TRUE)
table(iris[a[[1]], 5]) ## 10 values from each group
```

---

Greenacre's power transformation

*Greenacre's power transformation*

---

**Description**

Greenacre's power transformation.

**Usage**

```
green(x, theta)
```

**Arguments**

x	A matrix with the compositional data.
theta	The value of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\theta = 0$ the log transformation is applied.

**Details**

Greenacre's transformation is applied to the compositional data.

**Value**

A matrix with the power transformed data.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Greenacre, M. (2009). Power transformations in correspondence analysis. *Computational Statistics & Data Analysis*, 53(8): 3107-3116. <http://www.econ.upf.edu/~michael/work/PowerCA.pdf>

**See Also**

[alfa](#)

**Examples**

```
library(MASS)
x <- as.matrix(fg1[, 2:9])
x <- x / rowSums(x)
y1 <- green(x, 0.1)
y2 <- green(x, 0.2)
rbind( colMeans(y1), colMeans(y2) )
```

---

Helper Frechet mean for compositional data

*Helper Frechet mean for compositional data*

---

**Description**

Helper Frechet mean for compositional data.

**Usage**

```
frechet2(x, di, a, k)
```

**Arguments**

x	A matrix with the compositional data.
di	A matrix with indices as produced by the function "dista" of the package "Rfast" or the function "nn" of the package "Rnanoflann". Better see the details section.
a	The value of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ the isometric log-ratio transformation is applied and the closed geometric mean is calculated.
k	The number of nearest neighbours used for the computation of the Frechet means.

**Details**

The power transformation is applied to the compositional data and the mean vector is calculated. Then the inverse of it is calculated and the inverse of the power transformation applied to the last vector is the Frechet mean.

What this helper function do is to speed up the Frechet mean when used in the  $\alpha$ -k-NN regression. The  $\alpha$ -k-NN regression computes the Frechet mean of the k nearest neighbours for a value of  $\alpha$  and this function does exactly that. Suppose you want to predict the compositional value of some new predictors. For each predictor value you must use the Frechet mean computed at various nearest neighbours. This function performs these computations in a fast way. It is not the fastest way, yet it is a pretty fast way. This function is being called inside the function [aknn.reg](#).

**Value**

A list where each element contains a matrix. Each matrix contains the Frechet means computed at various nearest neighbours.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain. <https://arxiv.org/pdf/1106.1451.pdf>

**See Also**

[alfa](#), [alfainv](#), [profile](#)

**Examples**

```
library(MASS)
library(Rfast)
x <- as.matrix(fgl[, 2:9])
x <- x / rowSums(x)
xnew <- x[1:10, ]
x <- x[-c(1:10), ]
k <- 2:5
di <- Rfast::dista( xnew, x, k = max(k), index = TRUE, square = TRUE )
est <- frechet2(x, di, 0.2, k)
```

---

Helper functions for the Kullback-Leibler regression

*Helper functions for the Kullback-Leibler regression*

---

**Description**

Helper functions for the Kullback-Leibler regression.

**Usage**

```
kl.compreg2(y, x, con = TRUE, xnew = NULL, tol = 1e-07, maxiters = 50)
klcompreg.boot(y, x, der, der2, id, b1, n, p, d, tol = 1e-07, maxiters = 50)
```

**Arguments**

**y** A matrix with the compositional data (dependent variable). Zero values are allowed. For the `klcompreg.boot` the first column is removed.

**x** The predictor variable(s), they can be either continuous or categorical or both. In the `klcompreg.boot` this is the design matrix.

con	If this is TRUE (default) then the constant term is estimated, otherwise the model includes no constant term.
xnew	If you have new data use it, otherwise leave it NULL.
tol	The tolerance value to terminate the Newton-Raphson procedure.
maxiters	The maximum number of Newton-Raphson iterations.
der	An vector to put the first derivative there.
der2	An empty matrix to put the second derivatives there, the Hessian matrix will be put here.
id	A help vector with indices.
b1	The matrix with the initial estimated coefficients.
n	The sample size
p	The number of columns of the design matrix.
d	The dimensionality of the simplex, that is the number of columns of the compositional data minus 1.

### Details

These are help functions for the [kl.compreg](#) function. They are not to be called directly by the user.

### Value

For `kl.compreg2` a list including:

iters	The nubmer of iterations required by the Newton-Raphson.
loglik	The loglikelihood.
be	The beta coefficients.
est	The fitted or the predicted values (if <code>xnew</code> is not NULL).

For `klcompreg.boot` a list including:

loglik	The loglikelihood.
be	The beta coefficients.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

### References

Murteira, Jose MR, and Joaquim JS Ramalho 2016. Regression analysis of multivariate fractional data. *Econometric Reviews* 35(4): 515-552.

### See Also

[diri.reg](#), [js.compreg](#), [ols.compreg](#), [comp.reg](#)

**Examples**

```

library(MASS)
x <- as.vector(fgl[, 1])
y <- as.matrix(fgl[, 2:9])
y <- y / rowSums(y)
mod1<- kl.compreg(y, x, B = 1, ncores = 1)
mod2 <- js.compreg(y, x, B = 1, ncores = 1)

```

---

Hotelling's multivariate version of the 2 sample t-test for Euclidean data

*Hotelling's multivariate version of the 2 sample t-test for Euclidean data*

---

**Description**

Hotelling's test for testing the equality of two Euclidean population mean vectors.

**Usage**

```
hotel2T2(x1, x2, a = 0.05, R = 999, graph = FALSE)
```

**Arguments**

x1	A matrix containing the Euclidean data of the first group.
x2	A matrix containing the Euclidean data of the second group.
a	The significance level, set to 0.05 by default.
R	If R is 1 no bootstrap calibration is performed and the classical p-value via the F distribution is returned. If R is greater than 1, the bootstrap p-value is returned.
graph	A boolean variable which is taken into consideration only when bootstrap calibration is performed. IF TRUE the histogram of the bootstrap test statistic values is plotted.

**Details**

The first case scenario is when we assume equality of the two covariance matrices. This is called the two-sample Hotelling's  $T^2$  test (Mardia, Kent and Bibby, 1979, pg. 131-140) and Everitt (2005, pg. 139). The test statistic is defined as

$$T^2 = \frac{n_1 n_2}{n_1 + n_2} (\bar{\mathbf{X}}_1 - \bar{\mathbf{X}}_2)^T \mathbf{S}^{-1} (\bar{\mathbf{X}}_1 - \bar{\mathbf{X}}_2),$$

where  $\mathbf{S}$  is the pooled covariance matrix calculated under the assumption of equal covariance matrices  $\mathbf{S} = \frac{(n_1-1)\mathbf{S}_1 + (n_2-1)\mathbf{S}_2}{n_1+n_2-2}$ . Under  $H_0$  the statistic  $F$  given by

$$F = \frac{(n_1 + n_2 - p - 1) T^2}{(n_1 + n_2 - 2) p}$$



follows the  $F$  distribution with  $p$  and  $n_1 + n_2 - p - 1$  degrees of freedom. Similar to the one-sample test, an extra argument ( $R$ ) indicates whether bootstrap calibration should be used or not. If  $R=1$ , then the asymptotic theory applies, if  $R>1$ , then the bootstrap p-value will be applied and the number of re-samples is equal to  $R$ . The estimate of the common mean used in the bootstrap to transform the data under the null hypothesis the mean vector of the combined sample, of all the observations.

The built-in command `manova` does the same thing exactly. Try it, the asymptotic  $F$  test is what you have to see. In addition, this command allows for more mean vector hypothesis testing for more than two groups. I noticed this command after I had written my function and nevertheless as I mention in the introduction this document has an educational character as well.

### Value

A list including:

<code>mesoi</code>	The two mean vectors.
<code>info</code>	The test statistic, the p-value, the critical value and the degrees of freedom of the $F$ distribution (numerator and denominator). This is given if no bootstrap calibration is employed.
<code>pvalue</code>	The bootstrap p-value is bootstrap is employed.
<code>note</code>	A message informing the user that bootstrap calibration has been employed.
<code>runtime</code>	The runtime of the bootstrap calibration.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

### References

Everitt B. (2005). *An R and S-Plus Companion to Multivariate Analysis*. Springer.

Mardia K.V., Kent J.T. and Bibby J.M. (1979). *Multivariate Analysis*. London: Academic Press.

Tsagris M., Preston S. and Wood A.T.A. (2017). Nonparametric hypothesis testing for equality of means on the simplex. *Journal of Statistical Computation and Simulation*, 87(2): 406–422.

### See Also

`james`, `el.test2`, `eel.test2`

### Examples

```
hotel2T2( as.matrix(iris[1:25, 1:4]), as.matrix(iris[26:50, 1:4]) )
hotel2T2( as.matrix(iris[1:25, 1:4]), as.matrix(iris[26:50, 1:4]), R = 1 )
```

---

Hypothesis testing for two or more compositional mean vectors

*Hypothesis testing for two or more compositional mean vectors*

---

### Description

Hypothesis testing for two or more compositional mean vectors.

### Usage

```
comp.test(x, ina, test = "james", R = 0, ncores = 1, graph = FALSE)
```

### Arguments

x	A matrix containing compositional data.
ina	A numerical or factor variable indicating the groups of the data.
test	This can take the values of "james" for James' test, "hotel" for Hotelling's test, "maov" for multivariate analysis of variance assuming equality of the covariance matrices, "maovjames" for multivariate analysis of variance without assuming equality of the covariance matrices. "el" for empirical likelihood or "eel" for exponential empirical likelihood.
R	This depends upon the value of the argument "test". If the test is "maov" or "maovjames", R is not taken into consideration. If test is "hotel", then R denotes the number of bootstrap resamples. If test is "james", then R can be 1 (chi-square distribution), 2 ( F distribution), or more for bootstrap calibration. If test is "el", then R can be 0 (chi-square), 1 (corrected chi-sqaure), 2 (F distribution) or more for bootstrap calibration. See the help page of each test for more information.
ncores	How many to cores to use. This is taken into consideration only if test is "el" and R is more than 2.
graph	A boolean variable which is taken into consideration only when bootstrap calibration is performed. IF TRUE the histogram of the bootstrap test statistic values is plotted. This is taken into account only when R is greater than 2.

### Details

The idea is to apply the  $\alpha$ -transformation, with  $\alpha = 1$ , to the compositional data and then use a test to compare their mean vectors. See the help page of each test for more information. The function is visible so you can see exactly what is going on.

### Value

A list including:

result	The outcome of each test.
--------	---------------------------

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Giorgos Athineou <gioathineou@gmail.com>.

**References**

Tsagris M., Preston S. and Wood A.T.A. (2017). Nonparametric hypothesis testing for equality of means on the simplex. *Journal of Statistical Computation and Simulation*, 87(2): 406-422.

G.S. James (1954). Tests of Linear Hypotheses in Univariate and Multivariate Analysis when the Ratios of the Population Variances are Unknown. *Biometrika*, 41(1/2): 19-43

Krishnamoorthy K. and Yanping Xia (2006). On Selecting Tests for Equality of Two Normal Mean Vectors. *Multivariate Behavioral Research* 41(4): 533-548.

Owen A. B. (2001). *Empirical likelihood*. Chapman and Hall/CRC Press.

Owen A.B. (1988). Empirical likelihood ratio confidence intervals for a single functional. *Biometrika* 75(2): 237-249.

Amaral G.J.A., Dryden I.L. and Wood A.T.A. (2007). Pivotal bootstrap methods for k-sample problems in directional statistics and shape analysis. *Journal of the American Statistical Association* 102(478): 695-707.

Preston S.P. and Wood A.T.A. (2010). Two-Sample Bootstrap Hypothesis Tests for Three-Dimensional Labelled Landmark Data. *Scandinavian Journal of Statistics* 37(4): 568-587.

Jing Bing-Yi and Andrew TA Wood (1996). Exponential empirical likelihood is not Bartlett correctable. *Annals of Statistics* 24(1): 365-369.

**See Also**

[hd.meantest2](#), [dptest](#)

**Examples**

```
ina <- rep(1:2, each = 50)
x <- as.matrix(iris[1:100, 1:4])
x <- x/ rowSums(x)
comp.test( x, ina, test = "james" )
comp.test( x, ina, test = "hotel" )
comp.test( x, ina, test = "el" )
comp.test( x, ina, test = "eel" )
```

---

ICE plot for projection pursuit regression with compositional predictor variables

*ICE plot for projection pursuit regression with compositional predictor variables*

---

**Description**

ICE plot for projection pursuit regression with compositional predictor variables.

**Usage**

```
ice.pprcomp(model, x, k = 1, frac = 0.1, type = "log")
```

**Arguments**

model	The ppr model, the outcome of the <code>pprcomp</code> function.
x	A matrix with the compositional data. No zero values are allowed.
k	Which variable to select?.
frac	Fraction of observations to use. The default value is 0.1.
type	Either "alr" or "log" corresponding to the additive log-ratio transformation or the simple logarithm applied to the compositional data.

**Details**

This function implements the Individual Conditional Expectation plots of Goldstein et al. (2015). See the references for more details.

**Value**

A graph with several curves. The horizontal axis contains the selected variable, whereas the vertical axis contains the centered predicted values. The black curves are the effects for each observation and the blue line is their average effect.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

<https://christophm.github.io/interpretable-ml-book/ice.html>

Goldstein, A., Kapelner, A., Bleich, J. and Pitkin, E. (2015). Peeking inside the black box: Visualizing statistical learning with plots of individual conditional expectation. *Journal of Computational and Graphical Statistics* 24(1): 44-65.

Friedman, J. H. and Stuetzle, W. (1981). Projection pursuit regression. *Journal of the American Statistical Association*, 76, 817-823. doi: 10.2307/2287576.

**See Also**

[pprcomp](#), [pprcomp.tune](#), [ice.kernreg](#), [alfa.pcr](#), [lc.reg](#), [comp.ppr](#)

**Examples**

```
x <- as.matrix( iris[, 2:4] )
x <- x/ rowSums(x)
y <- iris[, 1]
model <- pprcomp(y, x)
ice <- ice.pprcomp(model, x, k = 1)
```

---

ICE plot for the alpha-k-NN regression

*ICE plot for the  $\alpha - k - NN$  regression*

---

**Description**

ICE plot for the  $\alpha - k - NN$  regression.

**Usage**

```
ice.aknnreg(y, x, a, k, apostasi = "euclidean", rann = FALSE,
ind = 1, frac = 0.2, qpos = 0.9)
```

**Arguments**

y	A numerical vector with the response values.
x	A numerical matrix with the predictor variables.
a	The value $\alpha$ to consider.
k	The number of nearest neighbours to consider.
apostasi	The type of distance to use, either "euclidean" or "manhattan".
rann	If you have large scale datasets and want a faster k-NN search, you can use kd-trees implemented in the R package "Rnanoflann". In this case you must set this argument equal to TRUE. Note however, that in this case, the only available distance is by default "euclidean".
ind	Which variable to select?.
frac	Fraction of observations to use. The default value is 0.1.
qpos	A number between 0.8 and 1. This is used to place the legend of the figure better. You can play with it. In the worst case scenario the code is open and you tweak this argument as you prefer.

**Details**

This function implements the Individual Conditional Expection plots of Goldstein et al. (2015). See the references for more details.

**Value**

A graph with several curves, one for each component. The horizontal axis contains the selected variable, whereas the vertical axis contains the locally smoothed predicted compositional lines.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

<https://christophm.github.io/interpretable-ml-book/ice.html>

Goldstein, A., Kapelner, A., Bleich, J. and Pitkin, E. (2015). Peeking inside the black box: Visualizing statistical learning with plots of individual conditional expectation. *Journal of Computational and Graphical Statistics* 24(1): 44-65.

**See Also**

[ice.akernreg](#), [ice.pprcomp](#)

**Examples**

```
y <- as.matrix( iris[, 2:4] )
x <- iris[, 1]
ice <- ice.aknreg(y, x, a = 0.6, k = 5, ind = 1)
```

---

ICE plot for the alpha-kernel regression  
*ICE plot for the  $\alpha$ -kernel regression*

---

**Description**

ICE plot for the  $\alpha$ -kernel regression.

**Usage**

```
ice.akernreg(y, x, a, h, type = "gauss", ind = 1, frac = 0.1, qpos = 0.9)
```

**Arguments**

y	A numerical vector with the response values.
x	A numerical matrix with the predictor variables.
a	The value $\alpha$ to consider.
h	The bandwidth value to consider.
type	The type of kernel to use, "gauss" or "laplace".
ind	Which variable to select?.
frac	Fraction of observations to use. The default value is 0.1.
qpos	A number between 0.8 and 1. This is used to place the legend of the figure better. You can play with it. In the worst case scenario the code is open and you tweak this argument as you prefer.

**Details**

This function implements the Individual Conditional Expectation plots of Goldstein et al. (2015). See the references for more details.

**Value**

A graph with several curves, one for each component. The horizontal axis contains the selected variable, whereas the vertical axis contains the locally smoothed predicted compositional lines.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

<https://christophm.github.io/interpretable-ml-book/ice.html>

Goldstein, A., Kapelner, A., Bleich, J. and Pitkin, E. (2015). Peeking inside the black box: Visualizing statistical learning with plots of individual conditional expectation. *Journal of Computational and Graphical Statistics* 24(1): 44-65.

**See Also**

[ice.aknnreg](#), [ice.pprcomp](#)

**Examples**

```
y <- as.matrix( iris[, 2:4] )
x <- iris[, 1]
ice <- ice.akernreg(y, x, a = 0.6, h = 0.1, ind = 1)
```

---

ICE plot for univariate kernel regression

*ICE plot for univariate kernel regression*

---

**Description**

ICE plot for univariate kernel regression.

**Usage**

```
ice.kernreg(y, x, h, type = "gauss", k = 1, frac = 0.1)
```

**Arguments**

y	A numerical vector with the response values.
x	A numerical matrix with the predictor variables.
h	The bandwidth value to consider.
type	The type of kernel to use, "gauss" or "laplace".
k	Which variable to select?.
frac	Fraction of observations to use. The default value is 0.1.

**Details**

This function implements the Individual Conditional Expectation plots of Goldstein et al. (2015). See the references for more details.

**Value**

A graph with several curves. The horizontal axis contains the selected variable, whereas the vertical axis contains the centered predicted values. The black curves are the effects for each observation and the blue line is their average effect.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

<https://christophm.github.io/interpretable-ml-book/ice.html>

Goldstein, A., Kapelner, A., Bleich, J. and Pitkin, E. (2015). Peeking inside the black box: Visualizing statistical learning with plots of individual conditional expectation. *Journal of Computational and Graphical Statistics* 24(1): 44-65.

**See Also**

[ice.pprcomp](#), [kernreg.tune](#), [alfa.pcr](#), [lc.reg](#)

**Examples**

```
x <- as.matrix( iris[, 2:4] )
y <- iris[, 1]
ice <- ice.kernreg(y, x, h = 0.1, k = 1)
```



---

Inverse of the alpha-transformation

*Inverse of the  $\alpha$ -transformation*

---

### Description

The inverse of the  $\alpha$ -transformation.

### Usage

```
alfainv(x, a, h = TRUE)
```

### Arguments

x	A matrix with Euclidean data. However, they must lie within the feasible, acceptable space. See references for more information.
a	The value of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ , the inverse of the isometric log-ratio transformation is applied.
h	If h = TRUE this means that the multiplication with the Helmer sub-matrix will take place. It is set to TRUE by default.

### Details

The inverse of the  $\alpha$ -transformation is applied to the data. If the data lie outside the  $\alpha$ -space, NAs will be returned for some values.

### Value

A matrix with the pairwise distances.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Giorgos Athineou <gioathineou@gmail.com>.

### References

- Tsagris M. and Stewart C. (2022). A Review of Flexible Transformations for Modeling Compositional Data. In *Advances and Innovations in Statistics and Data Science*, pp. 225–234. [https://link.springer.com/chapter/10.1007/978-3-031-08329-7\\_10](https://link.springer.com/chapter/10.1007/978-3-031-08329-7_10)
- Tsagris M.T., Preston S. and Wood A.T.A. (2016). Improved classification for compositional data using the  $\alpha$ -transformation. *Journal of Classification* 33(2): 243–261. <https://arxiv.org/pdf/1506.04976v2.pdf>
- Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In *Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain*. <https://arxiv.org/pdf/1106.1451.pdf>

**See Also**[alfa](#), [alfadist](#)**Examples**

```
library(MASS)
x <- as.matrix(fgl[1:10, 2:9])
x <- x / rowSums(x)
y <- alfa(x, 0.5)$aff
alfainv(y, 0.5)
```

---

 James multivariate version of the t-test

*James multivariate version of the t-test*

---

**Description**

James test for testing the equality of two population mean vectors without assuming equality of the covariance matrices.

**Usage**

```
james(y1, y2, a = 0.05, R = 999, graph = FALSE)
```

**Arguments**

y1	A matrix containing the Euclidean data of the first group.
y2	A matrix containing the Euclidean data of the second group.
a	The significance level, set to 0.05 by default.
R	If R is 1 no bootstrap calibration is performed and the classical p-value via the F distribution is returned. If R is greater than 1, the bootstrap p-value is returned.
graph	A boolean variable which is taken into consideration only when bootstrap calibration is performed. If TRUE the histogram of the bootstrap test statistic values is plotted.

**Details**

Here we show the modified version of the two-sample  $T^2$  test (function [hotel2T2](#)) in the case where the two covariances matrices cannot be assumed to be equal.

James (1954) proposed a test for linear hypotheses of the population means when the variances (or the covariance matrices) are not known. Its form for two  $p$ -dimensional samples is:

$$T_u^2 = (\bar{\mathbf{X}}_1 - \bar{\mathbf{X}}_2)^T \tilde{\mathbf{S}}^{-1} (\bar{\mathbf{X}}_1 - \bar{\mathbf{X}}_2),$$

where  $\tilde{\mathbf{S}} = \tilde{\mathbf{S}}_1 + \tilde{\mathbf{S}}_2 = \frac{\mathbf{S}_1}{n_1} + \frac{\mathbf{S}_2}{n_2}$ .

James (1954) suggested that the test statistic is compared with  $2h(\alpha)$ , a corrected  $\chi^2$  distribution whose form is

$$2h(\alpha) = \chi^2(A + B\chi^2),$$

where  $A = 1 + \frac{1}{2p} \sum_{i=1}^2 \frac{(\text{tr}\tilde{\mathbf{S}}^{-1}\tilde{\mathbf{S}}_i)^2}{n_i-1}$  and  $B = \frac{1}{p(p+2)} \left[ \sum_{i=1}^2 \frac{\text{tr}(\tilde{\mathbf{S}}^{-1}\tilde{\mathbf{S}}_i)^2}{n_i-1} + \frac{1}{2} \sum_{i=1}^2 \frac{(\text{tr}\tilde{\mathbf{S}}^{-1}\tilde{\mathbf{S}}_i)^2}{n_i-1} \right]$ .

If you want to do bootstrap to get the p-value, then you must transform the data under the null hypothesis. The estimate of the common mean is given by Aitchison (1986)

$$\hat{\boldsymbol{\mu}}_c = (n_1\mathbf{S}_1^{-1} + n_2\mathbf{S}_2^{-1})^{-1} (n_1\mathbf{S}_1^{-1}\bar{\mathbf{X}}_1 + n_2\mathbf{S}_2^{-1}\bar{\mathbf{X}}_2) = (\tilde{\mathbf{S}}_1^{-1} + \tilde{\mathbf{S}}_2^{-1})^{-1} (\tilde{\mathbf{S}}_1^{-1}\bar{\mathbf{X}}_1 + \tilde{\mathbf{S}}_2^{-1}\bar{\mathbf{X}}_2).$$

The modified Nel and van der Merwe (1986) test is based on the same quadratic form as that of James (1954) but the distribution used to compare the value of the test statistic is different. It is shown in Krishnamoorthy and Yanping (2006) that  $T_u^2 \sim \frac{\nu p}{\nu - p + 1} F_{p, \nu - p + 1}$  approximately, where

$$\nu = \frac{p+p^2}{\frac{1}{n_1} \{ \text{tr}[(\mathbf{S}_1\tilde{\mathbf{S}})^2] + \text{tr}[(\mathbf{S}_1\tilde{\mathbf{S}})]^2 \} + \frac{1}{n_2} \{ \text{tr}[(\mathbf{S}_2\tilde{\mathbf{S}})^2] + \text{tr}[(\mathbf{S}_2\tilde{\mathbf{S}})]^2 \}}.$$

The algorithm is taken by Krishnamoorthy and Yu (2004).

## Value

A list including:

note	A message informing the user about the test used.
mesoi	The two mean vectors.
info	The test statistic, the p-value, the correction factor and the corrected critical value of the chi-square distribution if the James test has been used or, the test statistic, the p-value, the critical value and the degrees of freedom (numerator and denominator) of the F distribution if the modified James test has been used.
pvalue	The bootstrap p-value if bootstrap is employed.
runtime	The runtime of the bootstrap calibration.

## Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

## References

- Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.
- James G.S. (1954). Tests of Linear Hypotheses in Univariate and Multivariate Analysis when the Ratios of the Population Variances are Unknown. *Biometrika*, 41(1/2): 19–43.
- Krishnamoorthy K. and Yu J. (2004). Modified Nel and Van der Merwe test for the multivariate Behrens-Fisher problem. *Statistics & Probability Letters*, 66(2): 161–169.
- Krishnamoorthy K. and Yanping Xia (2006). On Selecting Tests for Equality of Two Normal Mean Vectors. *Multivariate Behavioral Research*, 41(4): 533–548.
- Tsagris M., Preston S. and Wood A.T.A. (2017). Nonparametric hypothesis testing for equality of means on the simplex. *Journal of Statistical Computation and Simulation*, 87(2): 406–422.

**See Also**

[hotel2T2](#), [maovjames](#), [el.test2](#), [eel.test2](#)

**Examples**

```
james( as.matrix(iris[1:25, 1:4]), as.matrix(iris[26:50, 1:4]), R = 1 )
james( as.matrix(iris[1:25, 1:4]), as.matrix(iris[26:50, 1:4]), R = 2 )
james( as.matrix(iris[1:25, 1:4]), as.matrix(iris[26:50, 1:4]) )
```

---

Kernel regression with a numerical response vector or matrix

*Kernel regression with a numerical response vector or matrix*

---

**Description**

Kernel regression (Nadaraya-Watson estimator) with a numerical response vector or matrix.

**Usage**

```
kern.reg(xnew, y, x, h = seq(0.1, 1, length = 10), type = "gauss" )
```

**Arguments**

xnew	A matrix with the new predictor variables whose compositions are to be predicted.
y	A numerical vector or a matrix with the response value.
x	A matrix with the available predictor variables.
h	The bandwidth value(s) to consider.
type	The type of kernel to use, "gauss" or "laplace".

**Details**

The Nadaraya-Watson estimator regression is applied.

**Value**

The fitted values. If a single bandwidth is considered then this is a vector or a matrix, depending on the nature of the response. If multiple bandwidth values are considered then this is a matrix, if the response is a vector, or a list, if the response is a matrix.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Wand M. P. and Jones M. C. (1994). Kernel smoothing. CRC press.

**See Also**

[kernreg.tune](#), [ice.kernreg](#), [akern.reg](#), [aknn.reg](#)

**Examples**

```
y <- iris[, 1]
x <- iris[, 2:4]
est <- kern.reg(x, y, x, h = c(0.1, 0.2) )
```

---

Kullback-Leibler divergence and Bhattacharyya distance between two Dirichlet distributions

*Kullback-Leibler divergence and Bhattacharyya distance between two Dirichlet distributions*

---

**Description**

Kullback-Leibler divergence and Bhattacharyya distance between two Dirichlet distributions.

**Usage**

```
kl.diri(a, b, type = "KL")
```

**Arguments**

a	A vector with the parameters of the first Dirichlet distribution.
b	A vector with the parameters of the second Dirichlet distribution.
type	A variable indicating whether the Kullback-Leibler divergence ("KL") or the Bhattacharyya distance ("bhatt") is to be computed.

**Details**

Note that the order is important in the Kullback-Leibler divergence, since this is asymmetric, but not in the Bhattacharyya distance, since it is a metric.

**Value**

The value of the Kullback-Leibler divergence or the Bhattacharyya distance.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Ng Kai Wang, Guo-Liang Tian and Man-Lai Tang (2011). Dirichlet and related distributions: Theory, methods and applications. John Wiley & Sons.

**See Also**

[diri.est](#), [diri.nr](#)

**Examples**

```
library(MASS)
a <- runif(10, 0, 20)
b <- runif(10, 1, 10)
kl.diri(a, b)
kl.diri(b, a)
kl.diri(a, b, type = "bhatt")
kl.diri(b, a, type = "bhatt")
```

---

LASSO Kullback-Leibler divergence based regression

*LASSO Kullback-Leibler divergence based regression*

---

**Description**

LASSO Kullback-Leibler divergence based regression.

**Usage**

```
lasso.klcompreg(y, x, alpha = 1, lambda = NULL,
nlambda = 100, type = "grouped", xnew = NULL)
```

**Arguments**

<code>y</code>	A numerical matrix with compositional data. Zero values are allowed.
<code>x</code>	A numerical matrix containing the predictor variables.
<code>alpha</code>	The elastic net mixing parameter, with $0 \leq \alpha \leq 1$ . The penalty is defined as a weighted combination of the ridge and of the Lasso regression. When $\alpha = 1$ LASSO is applied, while $\alpha = 0$ yields the ridge regression.
<code>lambda</code>	<b>This information is copied from the package glmnet.</b> A user supplied lambda sequence. Typical usage is to have the program compute its own lambda sequence based on <code>nlambda</code> and <code>lambda.min.ratio</code> . Supplying a value of <code>lambda</code> overrides this. <b>WARNING:</b> use with care. Avoid supplying a single value for <code>lambda</code> (for predictions after CV use <code>predict()</code> instead). Supply instead a decreasing sequence of lambda values. <code>glmnet</code> relies on its warm starts for speed, and its often faster to fit a whole path than compute a single fit.
<code>nlambda</code>	<b>This information is copied from the package glmnet.</b> The number of <i>lambda</i> values, default is 100.

type	<b>This information is copied from the package glmnet.</b> If "grouped" then a grouped lasso penalty is used on the multinomial coefficients for a variable. This ensures they are all in our out together. The default in our case is "grouped".
xnew	If you have new data use it, otherwise leave it NULL.

### Details

The function uses the glmnet package to perform LASSO penalised regression. For more details see the function in that package.

### Value

A list including:

mod	We decided to keep the same list that is returned by glmnet. So, see the function in that package for more information.
est	If you supply a matrix in the "xnew" argument this will return an array of many matrices with the fitted values, where each matrix corresponds to each value of $\lambda$ .

### Author(s)

Michail Tsagris and Abdulaziz Alenazi.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Abdulaziz Alenazi <a.alenazi@nbu.edu.sa>.

### References

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

Alenazi A. A. (2022). f-divergence regression models for compositional data. Pakistan Journal of Statistics and Operation Research, 18(4): 867–882.

Friedman J., Hastie T. and Tibshirani R. (2010) Regularization Paths for Generalized Linear Models via Coordinate Descent. Journal of Statistical Software, Vol. 33(1), 1–22.

### See Also

[lassocoef.plot](#), [cv.lasso.klcompreg](#), [kl.compreg](#), [lasso.compreg](#), [ols.compreg](#), [alfa.pcr](#), [alfa.knn.reg](#)

### Examples

```
y <- as.matrix(iris[, 1:4])
y <- y / rowSums(y)
x <- matrix( rnorm(150 * 30), ncol = 30 )
a <- lasso.klcompreg(y, x)
```

---

LASSO log-ratio regression with compositional response

*LASSO log-ratio regression with compositional response*

---

## Description

LASSO log-ratio regression with compositional response.

## Usage

```
lasso.compreg(y, x, alpha = 1, lambda = NULL,
             nlambda = 100, xnew = NULL)
```

## Arguments

y	A numerical matrix with compositional data. Zero values are not allowed as the additive log-ratio transformation ( <a href="#">alr</a> ) is applied to the compositional response prior to implementing the LASSO algorithm.
x	A numerical matrix containing the predictor variables.
alpha	The elastic net mixing parameter, with $0 \leq \alpha \leq 1$ . The penalty is defined as a weighted combination of the ridge and of the Lasso regression. When $\alpha = 1$ LASSO is applied, while $\alpha = 0$ yields the ridge regression.
lambda	<b>This information is copied from the package glmnet.</b> A user supplied lambda sequence. Typical usage is to have the program compute its own lambda sequence based on nlambda and lambda.min.ratio. Supplying a value of lambda overrides this. <b>WARNING:</b> use with care. Avoid supplying a single value for lambda (for predictions after CV use predict() instead). Supply instead a decreasing sequence of lambda values. glmnet relies on its warm starts for speed, and its often faster to fit a whole path than compute a single fit.
nlambda	<b>This information is copied from the package glmnet.</b> The number of lambda values, default is 100.
xnew	If you have new data use it, otherwise leave it NULL.

## Details

The function uses the glmnet package to perform LASSO penalised regression. For more details see the function in that package.

## Value

A list including:

mod	We decided to keep the same list that is returned by glmnet. So, see the function in that package for more information.
est	If you supply a matrix in the "xnew" argument this will return an array of many matrices with the fitted values, where each matrix corresponds to each value of $\lambda$ .



**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

Friedman, J., Hastie, T. and Tibshirani, R. (2010) Regularization Paths for Generalized Linear Models via Coordinate Descent. Journal of Statistical Software, Vol. 33(1), 1-22.

**See Also**

[cv.lasso.compreg](#), [lassocoef.plot](#), [lasso.klcompreg](#), [cv.lasso.klcompreg](#), [comp.reg](#)

**Examples**

```
y <- as.matrix(iris[, 1:4])
y <- y / rowSums(y)
x <- matrix( rnorm(150 * 30), ncol = 30 )
a <- lasso.compreg(y, x)
```

---

LASSO with compositional predictors using the *alpha*-transformation

*LASSO with compositional predictors using the *alpha*-transformation*

---

**Description**

LASSO with compositional predictors using the *alpha*-transformation.

**Usage**

```
alfa.lasso(y, x, a = seq(-1, 1, by = 0.1), model = "gaussian", lambda = NULL,
xnew = NULL)
```

**Arguments**

<code>y</code>	A numerical vector or a matrix for multinomial logistic regression.
<code>x</code>	A numerical matrix containing the predictor variables, compositional data, where zero values are allowed..
<code>a</code>	A vector with a grid of values of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ the isometric log-ratio transformation is applied.
<code>model</code>	The type of the regression model, "gaussian", "binomial", "poisson", "multinomial", or "mgaussian".

lambda	<b>This information is copied from the package glmnet.</b> A user supplied lambda sequence. Typical usage is to have the program compute its own lambda sequence based on nlambdas and lambda.min.ratio. Supplying a value of lambda overrides this. <b>WARNING:</b> use with care. Avoid supplying a single value for lambda (for predictions after CV use predict() instead). Supply instead a decreasing sequence of lambda values. glmnet relies on its warm starts for speed, and is often faster to fit a whole path than compute a single fit.
xnew	If you have new data use it, otherwise leave it NULL.

**Details**

The function uses the glmnet package to perform LASSO penalised regression. For more details see the function in that package.

**Value**

A list including sublists for each value of  $\alpha$ :

mod	We decided to keep the same list that is returned by glmnet. So, see the function in that package for more information.
est	If you supply a matrix in the "xnew" argument this will return an array of many matrices with the fitted values, where each matrix corresponds to each value of $\lambda$ .

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

Friedman, J., Hastie, T. and Tibshirani, R. (2010) Regularization Paths for Generalized Linear Models via Coordinate Descent. Journal of Statistical Software, Vol. 33(1), 1–22.

**See Also**

[alfalasso.tune](#), [cv.lasso.klcompreg](#), [lasso.compreg](#), [alfa.knn.reg](#)

**Examples**

```
y <- as.matrix(iris[, 1])
x <- rdiri(150, runif(20, 2, 5) )
mod <- alfa.lasso(y, x, a = c(0, 0.5, 1))
```

---

Log-contrast GLMs with compositional predictor variables

*Log-contrast GLMS with compositional predictor variables*

---

### Description

Log-contrast GLMs with compositional predictor variables.

### Usage

```
lc.glm(y, x, z = NULL, model = "logistic", xnew = NULL, znew = NULL)
```

### Arguments

y	A numerical vector containing the response variable values. This is either a binary variable or a vector with counts.
x	A matrix with the predictor variables, the compositional data. No zero values are allowed.
z	A matrix, data.frame, factor or a vector with some other covariate(s).
model	For the <code>ulc.glm()</code> , this can be either "logistic" or "poisson".
xnew	A matrix containing the new compositional data whose response is to be predicted. If you have no new data, leave this NULL as is by default.
znew	A matrix, data.frame, factor or a vector with the values of some other covariate(s). If you have no new data, leave this NULL as is by default.

### Details

The function performs the log-contrast logistic or Poisson regression model. The logarithm of the compositional predictor variables is used (hence no zero values are allowed). The response variable is linked to the log-transformed data with the constraint that the sum of the regression coefficients equals 0. If you want the regression without the sum-to-zero constraints see [ulc.glm](#). Extra predictors variables are allowed as well, for instance categorical or continuous.

### Value

A list including:

devi	The residual deviance of the logistic or Poisson regression model.
be	The constrained regression coefficients. Their sum (excluding the constant) equals 0.
est	If the arguments "xnew" and znew were given these are the predicted or estimated values, otherwise it is NULL.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

**References**

- Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.
- Lu J., Shi P. and Li H. (2019). Generalized linear models with linear constraints for microbiome compositional data. *Biometrics*, 75(1): 235–244.

**See Also**

`ulc.glm`, `lc.glm2`, `ulc.glm2`, `lcglm.aov`

**Examples**

```
y <- rbinom(150, 1, 0.5)
x <- rdirich(150, runif(3, 1, 4) )
mod1 <- lc.glm(y, x)
```

---

Log-contrast logistic or Poisson regression with with multiple  
compositional predictors

*Log-contrast logistic or Poisson regression with with multiple compo-  
sitional predictors*

---

**Description**

Log-contrast logistic or Poisson regression with with multiple compositional predictors.

**Usage**

```
lc.glm2(y, x, z = NULL, model = "logistic", xnew = NULL, znew = NULL)
```

**Arguments**

- |                    |   |
|--------------------|---|
| <code>y</code>     | A numerical vector containing the response variable values. This is either a binary variable or a vector with counts.                           |
| <code>x</code>     | A matrix with the predictor variables, the compositional data. No zero values are allowed.  |
| <code>z</code>     | A matrix, data.frame, factor or a vector with some other covariate(s).  |
| <code>model</code> | This can be either "logistic" or "poisson".   |
| <code>xnew</code>  | A matrix containing the new compositional data whose response is to be predicted. If you have no new data, leave this NULL as is by default.    |
| <code>znew</code>  | A matrix, data.frame, factor or a vector with the values of some other covariate(s). If you have no new data, leave this NULL as is by default. |

## Details

The function performs the log-contrast logistic or Poisson regression model. The logarithm of the compositional predictor variables is used (hence no zero values are allowed). The response variable is linked to the log-transformed data with the constraint that the sum of the regression coefficients equals 0. If you want the regression without the sum-to-zero constraints see [ulc.glm2](#). Extra predictor variables are allowed as well, for instance categorical or continuous.

## Value

A list including:

<code>devi</code>	The residual deviance of the logistic or Poisson regression model.
<code>be</code>	The constrained regression coefficients. Their sum (excluding the constant) equals 0.
<code>est</code>	If the arguments "xnew" and "znew" were given these are the predicted or estimated values, otherwise it is NULL.

## Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

## References

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

Lu J., Shi P. and Li H. (2019). Generalized linear models with linear constraints for microbiome compositional data. *Biometrics*, 75(1): 235–244.

## See Also

[ulc.glm2](#), [ulc.glm](#), [lc.glm](#)

## Examples

```
y <- rbinom(150, 1, 0.5)
x <- list()
x1 <- as.matrix(iris[, 2:4])
x1 <- x1 / rowSums(x1)
x[[ 1 ]] <- x1
x[[ 2 ]] <- rdir(150, runif(4) )
x[[ 3 ]] <- rdir(150, runif(5) )
mod <- lc.glm2(y, x)
```

---

Log-contrast quantile regression with compositional predictor variables

*Log-contrast quantile regression with compositional predictor variables*

---

## Description

Log-contrast quantile regression with compositional predictor variables.

## Usage

```
lc.rq(y, x, z = NULL, tau, xnew = NULL, znew = NULL)
```

## Arguments

y	A numerical vector containing the response variable values.
x	A matrix with the predictor variables, the compositional data. No zero values are allowed.
z	A matrix, data.frame, factor or a vector with some other covariate(s).
tau	The quantile to be estimated, a number between 0 and 1.
xnew	A matrix containing the new compositional data whose response is to be predicted. If you have no new data, leave this NULL as is by default.
znew	A matrix, data.frame, factor or a vector with the values of some other covariate(s). If you have no new data, leave this NULL as is by default.

## Details

The function performs the quantile regression model. The logarithm of the compositional predictor variables is used (hence no zero values are allowed). The response variable is linked to the log-transformed data with the constraint that the sum of the regression coefficients equals 0. If you want the regression without the sum-to-zero constraints see [ulc.rq](#). Extra predictor variables are allowed as well, for instance categorical or continuous.

## Value

A list including:

mod	The object as returned by the function <code>quantreg::rq()</code> . This is useful for hypothesis testing purposes.
be	The constrained regression coefficients. Their sum (excluding the constant) equals 0.
est	If the arguments "xnew" and znew were given these are the predicted or estimated values, otherwise it is NULL.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

Koenker R. W. and Bassett G. W. (1978). Regression Quantiles, *Econometrica*, 46(1): 33–50.

Koenker R. W. and d'Orey V. (1987). Algorithm AS 229: Computing Regression Quantiles. *Applied Statistics*, 36(3): 383–393.

**See Also**

[lc.rq2](#), [ulc.rq](#)

**Examples**

```
y <- rnorm(150)
x <- rdir(150, runif(3, 1, 4) )
mod1 <- lc.rq(y, x)
```

---

Log-contrast quantile regression with with multiple compositional predictors

*Log-contrast quantile regression with with multiple compositional predictors*

---

**Description**

Log-contrast quantile regression with with multiple compositional predictors.

**Usage**

```
lc.rq2(y, x, z = NULL, tau = 0.5, xnew = NULL, znew = NULL)
```

**Arguments**

y	A numerical vector containing the response variable values.
x	A matrix with the predictor variables, the compositional data. No zero values are allowed.
z	A matrix, data.frame, factor or a vector with some other covariate(s).
tau	The quantile to be estimated, a number between 0 and 1.
xnew	A matrix containing the new compositional data whose response is to be predicted. If you have no new data, leave this NULL as is by default.
znew	A matrix, data.frame, factor or a vector with the values of some other covariate(s). If you have no new data, leave this NULL as is by default.

**Details**

The function performs the log-contrast quantile regression model. The logarithm of the compositional predictor variables is used (hence no zero values are allowed). The response variable is linked to the log-transformed data with the constraint that the sum of the regression coefficients equals 0. If you want the regression without the sum-to-zero constraints see [ulc.rq2](#). Extra predictor variables are allowed as well, for instance categorical or continuous.

**Value**

A list including:

<code>mod</code>	The object as returned by the function <code>quantreg::rq()</code> . This is useful for hypothesis testing purposes.
<code>be</code>	The constrained regression coefficients. Their sum (excluding the constant) equals 0.
<code>est</code>	If the arguments "xnew" and znew were given these are the predicted or estimated values, otherwise it is NULL.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

**References**

- Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.
- Koenker R. W. and Bassett G. W. (1978). Regression Quantiles, *Econometrica*, 46(1): 33–50.
- Koenker R. W. and d’Orey V. (1987). Algorithm AS 229: Computing Regression Quantiles. *Applied Statistics*, 36(3): 383–393.

**See Also**

[lc.rq](#), [ulc.rq](#)

**Examples**

```
y <- rnorm(150)
x <- list()
x1 <- as.matrix(iris[, 2:4])
x1 <- x1 / rowSums(x1)
x[[ 1 ]] <- x1
x[[ 2 ]] <- rdir(150, runif(4) )
x[[ 3 ]] <- rdir(150, runif(5) )
mod <- lc.rq2(y, x)
```



---

Log-contrast regression with compositional predictor variables

*Log-contrast regression with compositional predictor variables*

---

## Description

Log-contrast regression with compositional predictor variables.

## Usage

```
lc.reg(y, x, z = NULL, xnew = NULL, znew = NULL)
```

## Arguments

y	A numerical vector containing the response variable values. This must be a continuous variable.
x	A matrix with the predictor variables, the compositional data. No zero values are allowed.
z	A matrix, data.frame, factor or a vector with some other covariate(s).
xnew	A matrix containing the new compositional data whose response is to be predicted. If you have no new data, leave this NULL as is by default.
znew	A matrix, data.frame, factor or a vector with the values of some other covariate(s). If you have no new data, leave this NULL as is by default.

## Details

The function performs the log-contrast regression model as described in Aitchison (2003), pg. 84-85. The logarithm of the compositional predictor variables is used (hence no zero values are allowed). The response variable is linked to the log-transformed data with the constraint that the sum of the regression coefficients equals 0. Hence, we apply constrained least squares, which has a closed form solution. The constrained least squares is described in Chapter 8.2 of Hansen (2019). The idea is to minimise the sum of squares of the residuals under the constraint  $R^T \beta = c$ , where  $c = 0$  in our case. If you want the regression without the sum-to-zero constraints see [ulc.reg](#). Extra predictors variables are allowed as well, for instance categorical or continuous.

## Value

A list including:

be	The constrained regression coefficients. Their sum (excluding the constant) equals 0.
covbe	The covariance matrix of the constrained regression coefficients.
va	The estimated regression variance.
residuals	The vector of residuals.
est	If the arguments "xnew" and znew were given these are the predicted or estimated values, otherwise it is NULL.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

Hansen, B. E. (2022). Econometrics. Princeton University Press.

**See Also**

[ulc.reg](#), [lcreg.aov](#), [lc.reg2](#), [alfa.pcr](#), [alfa.knn.reg](#)

**Examples**

```
y <- iris[, 1]
x <- as.matrix(iris[, 2:4])
x <- x / rowSums(x)
mod1 <- lc.reg(y, x)
mod2 <- lc.reg(y, x, z = iris[, 5])
```

---

Log-contrast regression with multiple compositional predictors

*Log-contrast regression with multiple compositional predictors*

---

**Description**

Log-contrast regression with multiple compositional predictors.

**Usage**

```
lc.reg2(y, x, z = NULL, xnew = NULL, znew = NULL)
```

**Arguments**

y	A numerical vector containing the response variable values. This must be a continuous variable.
x	A list with multiple matrices with the predictor variables, the compositional data. No zero values are allowed.
z	A matrix, data.frame, factor or a vector with some other covariate(s).
xnew	A matrix containing a list with multiple matrices with compositional data whose response is to be predicted. If you have no new data, leave this NULL as is by default.
znew	A matrix, data.frame, factor or a vector with the values of some other covariate(s). If you have no new data, leave this NULL as is by default.

**Details**

The function performs the log-contrast regression model as described in Aitchison (2003), pg. 84-85. The logarithm of the compositional predictor variables is used (hence no zero values are allowed). The response variable is linked to the log-transformed data with the constraint that the sum of the regression coefficients for each composition equals 0. Hence, we apply constrained least squares, which has a closed form solution. The constrained least squares is described in Chapter 8.2 of Hansen (2019). The idea is to minimise the sum of squares of the residuals under the constraint  $R^T \beta = c$ , where  $c = 0$  in our case. If you want the regression without the sum-to-zero constraints see [ulc.reg2](#). Extra predictor variables are allowed as well, for instance categorical or continuous. The difference with [lc.reg](#) is that instead of one, there are multiple compositions treated as predictor variables.

**Value**

A list including:

be	The constrained regression coefficients. The sum of the sets of coefficients (excluding the constant) corresponding to each predictor composition sums to 0.
covbe	If covariance matrix of the constrained regression coefficients.
va	The variance of the estimated regression coefficients.
residuals	The vector of residuals.
est	If the arguments "xnew" and "znew" were given these are the predicted or estimated values, otherwise it is NULL.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

**References**

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

Hansen, B. E. (2022). Econometrics. Princeton University Press.

Xiaokang Liu, Xiaomei Cong, Gen Li, Kendra Maas and Kun Chen (2020). Multivariate Log-Contrast Regression with Sub-Compositional Predictors: Testing the Association Between Preterm Infants' Gut Microbiome and Neurobehavioral Outcome.

**See Also**

[ulc.reg2](#), [lc.reg](#), [ulc.reg](#), [lcreg.aov](#), [alfa.pcr](#), [alfa.knn.reg](#)

**Examples**

```
y <- iris[, 1]
x <- list()
x1 <- as.matrix(iris[, 2:4])
x1 <- x1 / rowSums(x1)
x[[ 1 ]] <- x1
```

```
x[[ 2 ]] <- rdiri(150, runif(4) )
x[[ 3 ]] <- rdiri(150, runif(5) )
mod <- lc.reg2(y, x)
be <- mod$be
sum(be[2:4])
sum(be[5:8])
sum(be[9:13])
```

---

Log-likelihood ratio test for a Dirichlet mean vector

*Log-likelihood ratio test for a Dirichlet mean vector*

---

### Description

Log-likelihood ratio test for a Dirichlet mean vector.

### Usage

```
dirimean.test(x, a)
```

### Arguments

x	A matrix with the compositional data. No zero values are allowed.
a	A compositional mean vector. The concentration parameter is estimated at first. If the elements do not sum to 1, it is assumed that the Dirichlet parameters are supplied.

### Details

Log-likelihood ratio test is performed for the hypothesis the given vector of parameters "a" describes the compositional data well.

### Value

If there are no zeros in the data, a list including:

param	A matrix with the estimated parameters under the null and the alternative hypothesis.
loglik	The log-likelihood under the alternative and the null hypothesis.
info	The value of the test statistic and its relevant p-value.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Giorgos Athineou <gioathineou@gmail.com>.

**References**

Ng Kai Wang, Guo-Liang Tian and Man-Lai Tang (2011). Dirichlet and related distributions: Theory, methods and applications. John Wiley & Sons.

**See Also**

[sym.test](#), [diri.nr](#), [diri.est](#), [rdiri](#), [ddiri](#)

**Examples**

```
x <- rdiri( 100, c(1, 2, 3) )
dirimean.test(x, c(1, 2, 3) )
dirimean.test( x, c(1, 2, 3)/6 )
```

---

Log-likelihood ratio test for a symmetric Dirichlet distribution  
*Log-likelihood ratio test for a symmetric Dirichlet distribution*

---

**Description**

Log-likelihood ratio test for a symmetric Dirichlet distribution.

**Usage**

```
sym.test(x)
```

**Arguments**

`x` A matrix with the compositional data. No zero values are allowed.

**Details**

Log-likelihood ratio test is performed for the hypothesis that all Dirichlet parameters are equal.

**Value**

A list including:

<code>est.par</code>	The estimated parameters under the alternative hypothesis.
<code>one.par</code>	The value of the estimated parameter under the null hypothesis.
<code>res</code>	The loglikelihood under the alternative and the null hypothesis, the value of the test statistic, its relevant p-value and the associated degrees of freedom, which are actually the dimensionality of the simplex, $D - 1$ , where $D$ is the number of components.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Ng Kai Wang, Guo-Liang Tian and Man-Lai Tang (2011). Dirichlet and related distributions: Theory, methods and applications. John Wiley & Sons.

**See Also**

[diri.nr](#), [diri.est](#), [rdiri](#), [dirimean.test](#)

**Examples**

```
x <- rdiri( 100, c(5, 7, 1, 3, 10, 2, 4) )
sym.test(x)
x <- rdiri( 100, c(5, 5, 5, 5, 5) )
sym.test(x)
```

---

Minimized Kullback-Leibler divergence between Dirichlet and logistic normal

*Minimized Kullback-Leibler divergence between Dirichlet and logistic normal*

---

**Description**

Minimized Kullback-Leibler divergence between Dirichlet and logistic normal distributions.

**Usage**

```
kl.diri.normal(a)
```

**Arguments**

**a** A vector with the parameters of the Dirichlet parameters.

**Details**

The function computes the minimized Kullback-Leibler divergence from the Dirichlet distribution to the logistic normal distribution.

**Value**

The minimized Kullback-Leibler divergence from the Dirichlet distribution to the logistic normal distribution.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Aitchison J. (1986). The statistical analysis of compositional data, p. 127. Chapman & Hall.

**See Also**

[diri.nr](#), [diri.contour](#), [rdiri](#), [ddiri](#), [dda](#), [diri.reg](#)

**Examples**

```
a <- runif(5, 1, 5)
kl.diri.normal(a)
```

---

Mixture model selection via BIC

*Mixture model selection via BIC*

---

**Description**

Mixture model selection via BIC.

**Usage**

```
bic.mixcompnorm(x, G, type = "alr", veo = FALSE, graph = TRUE)
```

**Arguments**

x	A matrix with compositional data.
G	A numeric vector with the number of components, clusters, to be considered, e.g. 1:3.
type	The type of transformation to be used, either the additive log-ratio ("alr"), the isometric log-ratio ("ilr") or the pivot coordinate ("pivot") transformation.
veo	Stands for "Variables exceed observations". If TRUE then if the number variables in the model exceeds the number of observations, but the model is still fitted.
graph	A boolean variable, TRUE or FALSE specifying whether a graph should be drawn or not.

**Details**

The alr or the ilr-transformation is applied to the compositional data first and then mixtures of multivariate Gaussian distributions are fitted. BIC is used to decide on the optimal model and number of components.

**Value**

A plot with the BIC of the best model for each number of components versus the number of components. A list including:

mod	A message informing the user about the best model.
BIC	The BIC values for every possible model and number of components.
optG	The number of components with the highest BIC.
optmodel	The type of model corresponding to the highest BIC.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Ryan P. Browne, Aisha ElSherbiny and Paul D. McNicholas (2018). mixture: Mixture Models for Clustering and Classification. R package version 1.5.

Ryan P. Browne and Paul D. McNicholas (2014). Estimating Common Principal Components in High Dimensions. *Advances in Data Analysis and Classification*, 8(2), 217-226.

Aitchison J. (1986). *The statistical analysis of compositional data*. Chapman & Hall.

**See Also**

[mix.compnorm](#), [mix.compnorm.contour](#), [rmixcomp](#), [bic.alfamixnorm](#)

**Examples**

```
x <- as.matrix( iris[, 1:4] )
x <- x/ rowSums(x)
bic.mixcompnorm(x, 1:3, type = "alr", graph = FALSE)
bic.mixcompnorm(x, 1:3, type = "ilr", graph = FALSE)
```

---

Mixture model selection with the alpha-transformation using BIC

*Mixture model selection with the  $\alpha$ -transformation using BIC*

---

**Description**

Mixture model selection with the  $\alpha$ -transformation using BIC.

**Usage**

```
bic.alfamixnorm(x, G, a = seq(-1, 1, by = 0.1), veo = FALSE, graph = TRUE)
```



**Arguments**

x	A matrix with compositional data.
G	A numeric vector with the number of components, clusters, to be considered, e.g. 1:3.
a	A vector with a grid of values of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ the isometric log-ratio transformation is applied.
veo	Stands for "Variables exceed observations". If TRUE then if the number variables in the model exceeds the number of observations, but the model is still fitted.
graph	A boolean variable, TRUE or FALSE specifying whether a graph should be drawn or not.

**Details**

The  $\alpha$ -transformation is applied to the compositional data first and then mixtures of multivariate Gaussian distributions are fitted. BIC is used to decide on the optimal model and number of components.

**Value**

A list including:

abic	A list that contains the matrices of all BIC values for all values of $\alpha$ .
optalpha	The value of $\alpha$ that leads to the highest BIC.
optG	The number of components with the highest BIC.
optmodel	The type of model corresponding to the highest BIC.

If graph is set equal to TRUE a plot with the BIC of the best model for each number of components versus the number of components and a list with the results of the Gaussian mixture model for each value of  $\alpha$ .

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

- Ryan P. Browne, Aisha ElSherbiny and Paul D. McNicholas (2018). mixture: Mixture Models for Clustering and Classification. R package version 1.5.
- Ryan P. Browne and Paul D. McNicholas (2014). Estimating Common Principal Components in High Dimensions. *Advances in Data Analysis and Classification*, 8(2), 217-226.
- Aitchison J. (1986). *The statistical analysis of compositional data*. Chapman & Hall.
- Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In *Proceedings of the 4th Compositional Data Analysis Workshop*, Girona, Spain. <https://arxiv.org/pdf/1106.1451.pdf>

**See Also**

[alfa.mix.norm](#), [mix.compnorm](#), [mix.compnorm.contour](#), [rmixcomp](#), [alfa](#), [alfa.knn](#), [alfa.rda](#), [comp.nb](#)

**Examples**

```
x <- as.matrix( iris[, 1:4] )
x <- x/ rowSums(x)
bic.alfamixnorm(x, 1:3, a = c(0.4, 0.5, 0.6), graph = FALSE)
```

---

MLE for the multivariate  $t$  distribution

*MLE for the multivariate  $t$  distribution*

---

**Description**

MLE of the parameters of a multivariate  $t$  distribution.

**Usage**

```
multitv(y, plot = FALSE)
```

**Arguments**

<code>y</code>	A matrix with continuous data.
<code>plot</code>	If <code>plot</code> is TRUE the value of the maximum log-likelihood as a function of the degrees of freedom is presented.

**Details**

The parameters of a multivariate  $t$  distribution are estimated. This is used by the functions [comp.den](#) and [bivt.contour](#).

**Value**

A list including:

<code>center</code>	The location estimate.
<code>scatter</code>	The scatter matrix estimate.
<code>df</code>	The estimated degrees of freedom.
<code>loglik</code>	The log-likelihood value.
<code>mesos</code>	The classical mean vector.
<code>covariance</code>	The classical covariance matrix.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Giorgos Athineou <gioathineou@gmail.com>.

**References**

Nadarajah, S. and Kotz, S. (2008). Estimation methods for the multivariate t distribution. *Acta Applicandae Mathematicae*, 102(1):99-118.

**See Also**

[bivt.contour](#), [comp.den](#)

**Examples**

```
x <- as.matrix(iris[, 1:4])
multivt(x)
```

---

MLE of distributions defined in the (0, 1) interval

*MLE of distributions defined in the (0, 1) interval*

---

**Description**

MLE of distributions defined in the (0, 1) interval.

**Usage**

```
beta.est(x, tol = 1e-07)
logitnorm.est(x)
hsecant01.est(x, tol = 1e-07)
kumar.est(x, tol = 1e-07)
unitweibull.est(x, tol = 1e-07, maxiters = 100)
ibeta.est(x, tol = 1e-07)
zillogitnorm.est(x)
```

**Arguments**

x	A numerical vector with proportions, i.e. numbers in (0, 1) (zeros and ones are not allowed).
tol	The tolerance level up to which the maximisation stops.
maxiters	The maximum number of iterations the Newton-Raphson algorithm will perform.

**Details**

Maximum likelihood estimation of the parameters of some distributions are performed, some of which use the Newton-Raphson. Some distributions and hence the functions do not accept zeros. "logitnorm.mle" fits the logistic normal, hence no Newton-Raphson is required and the "hypersecant01.mle" use the golden ratio search as is it faster than the Newton-Raphson (less computations). The "ziligitnorm.est" stands for the zero inflated logistic normal distribution. The "ibeta.est" fits the zero or the one inflated beta distribution.

**Value**

A list including:

iters	The number of iterations required by the Newton-Raphson.
loglik	The value of the log-likelihood.
param	The estimated parameters. In the case of "hypersecant01.est" this is called "theta" as there is only one parameter.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Kumaraswamy, P. (1980). A generalized probability density function for double-bounded random processes. *Journal of Hydrology*. 46(1-2): 79-88.

Jones, M.C. (2009). Kumaraswamy's distribution: A beta-type distribution with some tractability advantages. *Statistical Methodology*. 6(1): 70-81.

You can also check the relevant wikipedia pages.

**See Also**

[diri.est](#)

**Examples**

```
x <- rbeta(1000, 1, 4)
beta.est(x)
ibeta.est(x)

x <- runif(1000)
hsecant01.est(x)
logitnorm.est(x)
ibeta.est(x)

x <- rbeta(1000, 2, 5)
x[sample(1:1000, 50)] <- 0
ibeta.est(x)
```

---

MLE of the Dirichlet distribution

*MLE of the a Dirichlet distribution*

---

### Description

MLE of the parameters of a Dirichlet distribution.

### Usage

```
diri.est(x, type = "mle")
```

### Arguments

x	A matrix containing compositional data.
type	If you want to estimate the parameters use type="mle". If you want to estimate the mean vector along with the precision parameter, the second parametrisation of the Dirichlet, use type="prec".

### Details

Maximum likelihood estimation of the parameters of a Dirichlet distribution is performed.

### Value

A list including:

loglik	The value of the log-likelihood.
param	The estimated parameters.
phi	The estimated precision parameter, if type = "prec".
mu	The estimated mean vector, if type = "prec".
runtime	The run time of the maximisation procedure.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Giorgos Athineou <gioathineou@gmail.com>.

### References

Ng Kai Wang, Guo-Liang Tian and Man-Lai Tang (2011). Dirichlet and related distributions: Theory, methods and applications. John Wiley & Sons.

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

**See Also**

[diri.nr](#), [diri.contour](#), [rdiri](#), [ddiri](#), [dda](#), [diri.reg](#)

**Examples**

```
x <- rdiri( 100, c(5, 7, 1, 3, 10, 2, 4) )
diri.est(x)
diri.est(x, type = "prec")
```

---

MLE of the Dirichlet distribution via Newton-Rapshon

*MLE of the Dirichlet distribution via Newton-Rapshon*

---

**Description**

MLE of the Dirichlet distribution via Newton-Rapshon.

**Usage**

```
diri.nr(x, type = 1, tol = 1e-07)
```

**Arguments**

<code>x</code>	A matrix containing compositional data. Zeros are not allowed.
<code>type</code>	Type can either be 1, so that the Newton-Rapshon is used for the maximisation of the log-likelihood, as Minka (2012) suggested or it can be 1. In the latter case the Newton-Rapshon algorithm is implemented involving matrix inversions. In addition an even faster implementation has been implemented (in C++) in the package <b>Rfast</b> and is used here.
<code>tol</code>	The tolerance level indicating no further increase in the log-likelihood.

**Details**

Maximum likelihood estimation of the parameters of a Dirichlet distribution is performed via Newton-Rapshon. Initial values suggested by Minka (2003) are used. The estimation is super faster than "diri.est" and the difference becomes really apparent when the sample size and or the dimensions increase. In fact this will work with millions of observations. So in general, I trust this one more than "diri.est".

The only problem I have seen with this method is that if the data are concentrated around a point, say the center of the simplex, it will be hard for this and the previous methods to give estimates of the parameters. In this extremely difficult scenario I would suggest the use of the previous function with the precision parametrization "diri.est(x, type = "prec")". It will be extremely fast and accurate.

**Value**

A list including:

<code>iter</code>	The number of iterations required. If the argument "type" is set to 2 this is not returned.
<code>loglik</code>	The value of the log-likelihood.
<code>param</code>	The estimated parameters.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Thomas P. Minka (2003). Estimating a Dirichlet distribution. <http://research.microsoft.com/en-us/um/people/minka/papers/dirichlet/minka-dirichlet.pdf>

**See Also**

[diri.est](#), [diri.contour](#) [rdiri](#), [ddiri](#), [dda](#)

**Examples**

```
x <- rdiri( 100, c(5, 7, 5, 8, 10, 6, 4) )
diri.nr(x)
diri.nr(x, type = 2)
diri.est(x)
```

---

MLE of the folded model for a given value of alpha

*MLE of the folded model for a given value of  $\alpha$*

---

**Description**

MLE of the folded model for a given value of  $\alpha$ .

**Usage**

```
alpha.mle(x, a)
a.mle(a, x)
```

**Arguments**

<code>x</code>	A matrix with the compositional data. No zero values are allowed.
<code>a</code>	A value of $\alpha$ .

**Details**

This is a function for choosing or estimating the value of  $\alpha$  in the  $\alpha$ -folded model (Tsagris and Stewart, 2020). It is called by [a.est](#).

**Value**

If "alpha.mle" is called, a list including:

<code>iters</code>	The number of iterations the EM algorithm required.
<code>loglik</code>	The maximized log-likelihood of the folded model.
<code>p</code>	The estimated probability inside the simplex of the $\alpha$ -folded model.
<code>mu</code>	The estimated mean vector of the $\alpha$ -folded model.
<code>su</code>	The estimated covariance matrix of the $\alpha$ -folded model.

If "a.mle" is called, the log-likelihood is returned only.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

**References**

Tsagris M. and Stewart C. (2022). A Review of Flexible Transformations for Modeling Compositional Data. In *Advances and Innovations in Statistics and Data Science*, pp. 225–234. [https://link.springer.com/chapter/10.1007/978-3-031-08329-7\\_10](https://link.springer.com/chapter/10.1007/978-3-031-08329-7_10)

Tsagris M. and Stewart C. (2020). A folded model for compositional data analysis. *Australian and New Zealand Journal of Statistics*, 62(2): 249-277. <https://arxiv.org/pdf/1802.07330.pdf>

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In *Proceedings of the 4th Compositional Data Analysis Workshop*, Girona, Spain. <https://arxiv.org/pdf/1106.1451.pdf>

**See Also**

[alfa.profile](#), [alfa](#), [alfainv](#), [a.est](#)

**Examples**

```
x <- as.matrix(iris[, 1:4])
x <- x / rowSums(x)
mod <- alfa.tune(x)
mod
alpha.mle(x, mod[1])
```



---

MLE of the zero adjusted Dirichlet distribution

*MLE of the zero adjusted Dirichlet distribution*

---

### Description

MLE of the zero adjusted Dirichlet distribution.

### Usage

```
zad.est(y)
```

### Arguments

`y` A matrix with the compositional data.

### Details

A zero adjusted Dirichlet distribution is being fitted and its parameters are estimated.

### Value

A list including:

<code>loglik</code>	The value of the log-likelihood.
<code>phi</code>	The precision parameter. If covariates are linked with it (function "diri.reg2"), this will be a vector.
<code>mu</code>	The mean vector of the distribution.
<code>runtime</code>	The time required by the model..

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

### References

Tsagris M. and Stewart C. (2018). A Dirichlet regression model for compositional data with zeros. *Lobachevskii Journal of Mathematics*, 39(3): 398–412.

Preprint available from <https://arxiv.org/pdf/1410.5011.pdf>

### See Also

[zadr](#), [diri.nr](#), [zilogitnorm.est](#), [zeroreplace](#)

**Examples**

```

y <- as.matrix(iris[, 1:3])
y <- y / rowSums(y)
mod1 <- diri.nr(y)
y[sample(1:450, 15) ] <- 0
mod2 <- zad.est(y)

```

---

Multivariate analysis of variance (James test)

*Multivariate analysis of variance (James test)*

---

**Description**

Multivariate analysis of variance without assuming equality of the covariance matrices.

**Usage**

```
maovjames(x, ina, a = 0.05)
```

**Arguments**

**x** A matrix containing Euclidean data.  
**ina** A numerical or factor variable indicating the groups of the data.  
**a** The significance level, set to 0.005 by default.

**Details**

James (1954) also proposed an alternative to MANOVA when the covariance matrices are not assumed equal. The test statistic for  $k$  samples is

$$J = \sum_{i=1}^k (\bar{\mathbf{x}}_i - \bar{\mathbf{X}})^T \mathbf{W}_i (\bar{\mathbf{x}}_i - \bar{\mathbf{X}}),$$

where  $\bar{\mathbf{x}}_i$  and  $n_i$  are the sample mean vector and sample size of the  $i$ -th sample respectively and  $\mathbf{W}_i = \left(\frac{\mathbf{S}_i}{n_i}\right)^{-1}$ , where  $\mathbf{S}_i$  is the covariance matrix of the  $i$ -sample mean vector and  $\bar{\mathbf{X}}$  is the estimate of the common mean  $\bar{\mathbf{X}} = \left(\sum_{i=1}^k \mathbf{W}_i\right)^{-1} \sum_{i=1}^k \mathbf{W}_i \bar{\mathbf{x}}_i$ .

Normally one would compare the test statistic with a  $\chi^2_{r,1-\alpha}$ , where  $r = p(k-1)$  are the degrees of freedom with  $k$  denoting the number of groups and  $p$  the dimensionality of the data. There are  $r$  constraints (how many univariate means must be equal, so that the null hypothesis, that all the mean vectors are equal, holds true), that is where these degrees of freedom come from. James (1954) compared the test statistic with a corrected  $\chi^2$  distribution instead. Let  $A$  and  $B$  be  $A = 1 + \frac{1}{2r} \sum_{i=1}^k \frac{[\text{tr}(\mathbf{I}_p - \mathbf{W}^{-1} \mathbf{W}_i)]^2}{n_i - 1}$  and  $B = \frac{1}{r(r+2)} \sum_{i=1}^k \left\{ \frac{\text{tr}[(\mathbf{I}_p - \mathbf{W}^{-1} \mathbf{W}_i)^2]}{n_i - 1} + \frac{[\text{tr}(\mathbf{I}_p - \mathbf{W}^{-1} \mathbf{W}_i)]^2}{2(n_i - 1)} \right\}$ .

The corrected quantile of the  $\chi^2$  distribution is given as before by  $2h(\alpha) = \chi^2(A + B\chi^2)$ .

**Value**

A vector with the next 4 elements:

<code>test</code>	The test statistic.
<code>correction</code>	The value of the correction factor.
<code>corr.critical</code>	The corrected critical value of the chi-square distribution.
<code>p-value</code>	The p-value of the corrected test statistic.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

James G.S. (1954). Tests of Linear Hypotheses in Univariate and Multivariate Analysis when the Ratios of the Population Variances are Unknown. *Biometrika*, 41(1/2): 19–43.

**See Also**

[hotel2T2](#), [james](#)

**Examples**

```
maovjames( as.matrix(iris[,1:4]), iris[,5] )
```

---

Multivariate analysis of variance assuming equality of the covariance matrices

*Multivariate analysis of variance assuming equality of the covariance matrices*

---

**Description**

Multivariate analysis of variance assuming equality of the covariance matrices.

**Usage**

```
maov(x, ina)
```

**Arguments**

<code>x</code>	A matrix containing Euclidean data.
<code>ina</code>	A numerical or factor variable indicating the groups of the data.

**Details**

Multivariate analysis of variance assuming equality of the covariance matrices.

**Value**

A list including:

note	A message stating whether the $F$ or the $chi^2$ approximation has been used.
result	The test statistic and the p-value.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Johnson R.A. and Wichern D.W. (2007, 6th Edition). Applied Multivariate Statistical Analysis, pg. 302–303.

Todorov V. and Filzmoser P. (2010). Robust Statistic for the One-way MANOVA. Computational Statistics & Data Analysis, 54(1): 37–48.

**See Also**

[maovjames](#), [hotel2T2](#), [james](#)

**Examples**

```
maov( as.matrix(iris[,1:4]), iris[,5] )
maovjames( as.matrix(iris[,1:4]), iris[,5] )
```

---

Multivariate kernel density estimation  
*Multivariate kernel density estimation*

---

**Description**

Multivariate kernel density estimation.

**Usage**

```
mkde(x, h = NULL, thumb = "silverman")
```

**Arguments**

x	A matrix with Euclidean (continuous) data.
h	The bandwidth value. It can be a single value, which is turned into a vector and then into a diagonal matrix, or a vector which is turned into a diagonal matrix. If you put this NULL then you need to specify the "thumb" argument below.
thumb	Do you want to use a rule of thumb for the bandwidth parameter? If no, set h equal to NULL and put "estim" for maximum likelihood cross-validation, "scott" or "silverman" for Scott's and Silverman's rules of thumb respectively.

**Details**

The multivariate kernel density estimate is calculated with a (not necessarily given) bandwidth value.

**Value**

A vector with the density estimates calculated for every vector.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Giorgos Athineou <gioathineou@gmail.com>.

**References**

Arsalane Chouaib Guidoum (2015). Kernel Estimator and Bandwidth Selection for Density and its Derivatives. The *kedd* R package.

M.P. Wand and M.C. Jones (1995). Kernel smoothing, pages 91-92.

B.W. Silverman (1986). Density estimation for statistics and data analysis, pages 76-78.

**See Also**

[mkde.tune](#), [comp.kerncontour](#)

**Examples**

```
mkde( as.matrix(iris[, 1:4]), thumb = "scott" )
mkde( as.matrix(iris[, 1:4]), thumb = "silverman" )
```

---

Multivariate kernel density estimation for compositional data

*Multivariate kernel density estimation for compositional data*

---

### Description

Multivariate kernel density estimation for compositional data.

### Usage

```
comp.kern(x, type= "alr", h = NULL, thumb = "silverman")
```

### Arguments

x	A matrix with Euclidean (continuous) data.
type	The type of transformation used, either the additive log-ratio ("alr"), the isometric log-ratio ("ilr") or the pivot coordinate ("pivot") transformation.
h	The bandwidth value. It can be a single value, which is turned into a vector and then into a diagonal matrix, or a vector which is turned into a diagonal matrix. If it is NULL, then you need to specify the "thumb" argument below.
thumb	Do you want to use a rule of thumb for the bandwidth parameter? If no, leave the "h" NULL and put "estim" for maximum likelihood cross-validation, "scott" or "silverman" for Scott's and Silverman's rules of thumb respectively.

### Details

The multivariate kernel density estimate is calculated with a (not necessarily given) bandwidth value.

### Value

A vector with the density estimates calculated for every vector.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

### References

Arsalane Chouaib Guidoum (2015). Kernel Estimator and Bandwidth Selection for Density and its Derivatives.

The kedd R package.

M.P. Wand and M.C. Jones (1995). Kernel smoothing, pages 91-92.

B.W. Silverman (1986). Density estimation for statistics and data analysis, pages 76-78.

**See Also**

[comp.kerncontour](#), [mkde](#)

**Examples**

```
x <- as.matrix(iris[, 1:3])
x <- x / rowSums(x)
f <- comp.kern(x)
```

---

Multivariate linear regression  
*Multivariate linear regression*

---

**Description**

Multivariate linear regression.

**Usage**

```
multivreg(y, x, plot = TRUE, xnew = NULL)
```

**Arguments**

y	A matrix with the Euclidean (continuous) data.
x	A matrix with the predictor variable(s), they have to be continuous.
plot	Should a plot appear or not?
xnew	If you have new data use it, otherwise leave it NULL.

**Details**

The classical multivariate linear regression model is obtained.

**Value**

A list including:

suma	A summary as produced by <a href="#">lm</a> , which includes the coefficients, their standard error, t-values, p-values.
r.squared	The value of the $R^2$ for each univariate regression.
resid.out	A vector with number indicating which vectors are potential residual outliers.
x.leverage	A vector with number indicating which vectors are potential outliers in the predictor variables space.
out	A vector with number indicating which vectors are potential outliers in the residuals and in the predictor variables space.
est	The predicted values if xnew is not NULL.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Giorgos Athineou <gioathineou@gmail.com>.

**References**

K.V. Mardia, J.T. Kent and J.M. Bibby (1979). Multivariate Analysis. Academic Press.

**See Also**

[diri.reg](#), [js.compreg](#), [kl.compreg](#), [ols.compreg](#), [comp.reg](#)

**Examples**

```
library(MASS)
x <- as.matrix(iris[, 1:2])
y <- as.matrix(iris[, 3:4])
multivreg(y, x, plot = TRUE)
```

---

Multivariate normal random values simulation on the simplex

*Multivariate normal random values simulation on the simplex*

---

**Description**

Multivariate normal random values simulation on the simplex.

**Usage**

```
rcompnorm(n, m, s, type = "alr")
```

**Arguments**

n	The sample size, a numerical value.
m	The mean vector in $R^d$ .
s	The covariance matrix in $R^d$ .
type	The alr (type = "alr") or the ilr (type = "ilr") is to be used for closing the Euclidean data onto the simplex.

**Details**

The algorithm is straightforward, generate random values from a multivariate normal distribution in  $R^d$  and brings the values to the simplex  $S^d$  using the inverse of a log-ratio transformation.



## Value

A matrix with the simulated data.

## Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

## References

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

## See Also

[comp.den](#), [rdiri](#), [rcompt](#), [rcompsn](#)

## Examples

```
x <- as.matrix(iris[, 1:2])
m <- colMeans(x)
s <- var(x)
y <- rcompnorm(100, m, s)
comp.den(y)
ternary(y)
```

---

Multivariate or univariate regression with compositional data in the covariates side using the alpha-transformation

*Multivariate or univariate regression with compositional data in the covariates side using the  $\alpha$ -transformation*

---

## Description

Multivariate or univariate regression with compositional data in the covariates side using the  $\alpha$ -transformation.

## Usage

```
alfa.pcr(y, x, a, k, model = "gaussian", xnew = NULL)
```

## Arguments

**y** A numerical vector containing the response variable values. They can be continuous, binary, discrete (counts). This can also be a vector with discrete values or a factor for the multinomial regression (model = "multinomial").

**x** A matrix with the predictor variables, the compositional data.

a	The value of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ the isometric log-ratio transformation is applied.
k	How many principal components to use. You may also specify a vector and in this case the results produced will refer to each number of principal components.
model	The type of regression model to fit. The possible values are "gaussian", "multinomial", "binomial" and "poisson".
xnew	A matrix containing the new compositional data whose response is to be predicted. If you have no new data, leave this NULL as is by default.

### Details

The  $\alpha$ -transformation is applied to the compositional data first, the first  $k$  principal component scores are calculated and used as predictor variables for a regression model. The family of distributions can be either, "normal" for continuous response and hence normal distribution, "binomial" corresponding to binary response and hence logistic regression or "poisson" for count response and poisson regression.

### Value

A list including:

be	If linear regression was fitted, the regression coefficients of the $k$ principal component scores on the response variable $y$ .
mod	If another regression model was fitted its outcome as produced in the package <b>Rfast</b> .
per	The percentage of variance explained by the first $k$ principal components.
vec	The first $k$ principal components, loadings or eigenvectors. These are useful for future prediction in the sense that one needs not fit the whole model again.
est	If the argument "xnew" was given these are the predicted or estimated values (if xnew is not NULL). If the argument $k$ is a vector then this is a matrix with the estimated values for each number of components.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

### References

- Tsagris M. (2015). Regression analysis with compositional data containing zero values. *Chilean Journal of Statistics*, 6(2): 47-57. <https://arxiv.org/pdf/1508.01913v1.pdf>
- Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In *Proceedings of the 4th Compositional Data Analysis Workshop*, Girona, Spain. <https://arxiv.org/pdf/1106.1451.pdf>

**See Also**

[glm.pcr](#), [alfapcr.tune](#)

**Examples**

```
library(MASS)
y <- as.vector(fg1[, 1])
x <- as.matrix(fg1[, 2:9])
x <- x / rowSums(x)
mod <- alfa.pcr(y = y, x = x, 0.7, 1)
mod
```

---

Multivariate regression with compositional data

*Multivariate regression with compositional data*

---

**Description**

Multivariate regression with compositional data.

**Usage**

```
comp.reg(y, x, type = "classical", xnew = NULL, yb = NULL)
```

**Arguments**

<code>y</code>	A matrix with compositional data. Zero values are not allowed.
<code>x</code>	The predictor variable(s), they have to be continuous.
<code>type</code>	The type of regression to be used, "classical" for standard multivariate regression, or "spatial" for the robust spatial median regression. Alternatively you can type "lmfit" for the fast classical multivariate regression that does not return standard errors whatsoever.
<code>xnew</code>	This is by default set to NULL. If you have new data whose compositional data values you want to predict, put them here.
<code>yb</code>	If you have already transformed the data using the additive log-ratio transformation, put it here. Otherwise leave it NULL. This is intended to be used in the function <a href="#">alfareg.tune</a> in order to speed up the process.

**Details**

The additive log-ratio transformation is applied and then the chosen multivariate regression is implemented. The alr is easier to explain than the ilr and that is why the latter is avoided here.

**Value**

A list including:

runtime	The time required by the regression.
be	The beta coefficients.
seb	The standard error of the beta coefficients.
est	The fitted values of xnew if xnew is not NULL.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Giorgos Athineou <gioathineou@gmail.com>.

**References**

- Mardia K.V., Kent J.T., and Bibby J.M. (1979). Multivariate analysis. Academic press.  
Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

**See Also**

[multivreg](#), [spatmed.reg](#), [js.compreg](#), [diri.reg](#)

**Examples**

```
library(MASS)
y <- as.matrix(iris[, 1:3])
y <- y / rowSums(y)
x <- as.vector(iris[, 4])
mod1 <- comp.reg(y, x)
mod2 <- comp.reg(y, x, type = "spatial")
```

---

Multivariate skew normal random values simulation on the simplex  
*Multivariate skew normal random values simulation on the simplex*

---

**Description**

Multivariate skew normal random values simulation on the simplex.

**Usage**

```
rcompsn(n, xi, Omega, alpha, dp = NULL, type = "alr")
```

**Arguments**

n	The sample size, a numerical value.
xi	A numeric vector of length $d$ representing the location parameter of the distribution.
Omega	A $d \times d$ symmetric positive-definite matrix of dimension.
alpha	A numeric vector which regulates the slant of the density.
dp	A list with three elements, corresponding to xi, Omega and alpha described above. The default value is FALSE. If dp is assigned, individual parameters must not be specified.
type	The alr (type = "alr") or the ilr (type = "ilr") is to be used for closing the Euclidean data onto the simplex.

**Details**

The algorithm is straightforward, generate random values from a multivariate t distribution in  $R^d$  and brings the values to the simplex  $S^d$  using the inverse of a log-ratio transformation.

**Value**

A matrix with the simulated data.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Azzalini, A. and Dalla Valle, A. (1996). The multivariate skew-normal distribution. *Biometrika*, 83(4): 715-726.

Azzalini, A. and Capitanio, A. (1999). Statistical applications of the multivariate skew normal distribution. *Journal of the Royal Statistical Society Series B*, 61(3):579-602. Full-length version available from <http://arXiv.org/abs/0911.2093>

Aitchison J. (1986). *The statistical analysis of compositional data*. Chapman & Hall.

**See Also**

[comp.den](#), [rdiri](#), [rcompnorm](#)

**Examples**

```
x <- as.matrix(iris[, 1:2])
par <- sn::msn.mle(y = x)$dp
y <- rcompsn(100, dp = par)
comp.den(y, dist = "skewnorm")
ternary(y)
```

Multivariate  $t$  random values simulation on the simplex

*Multivariate  $t$  random values simulation on the simplex*

---

### Description

Multivariate  $t$  random values simulation on the simplex.

### Usage

```
rcompt(n, m, s, dof, type = "alr")
```

### Arguments

n	The sample size, a numerical value.
m	The mean vector in $R^d$ .
s	The covariance matrix in $R^d$ .
dof	The degrees of freedom.
type	The alr (type = "alr") or the ilr (type = "ilr") is to be used for closing the Euclidean data onto the simplex.

### Details

The algorithm is straightforward, generate random values from a multivariate  $t$  distribution in  $R^d$  and brings the values to the simplex  $S^d$  using the inverse of a log-ratio transformation.

### Value

A matrix with the simulated data.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

### References

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

### See Also

[comp.den](#), [rdiri](#), [rcompnorm](#)

**Examples**

```
x <- as.matrix(iris[, 1:2])
m <- Rfast::colmeans(x)
s <- var(x)
y <- rcompt(100, m, s, 10)
comp.den(y, dist = "t")
ternary(y)
```

---

Naive Bayes classifiers for compositional data

*Naive Bayes classifiers for compositional data*

---

**Description**

Naive Bayes classifiers for compositional data.

**Usage**

```
comp.nb(xnew = NULL, x, ina, type = "beta")
```

**Arguments**

xnew	A matrix with the new compositional predictor data whose class you want to predict. Zeros are not allowed
x	A matrix with the available compositional predictor data. Zeros are not allowed
ina	A vector of data. The response variable, which is categorical (factor is acceptable).
type	The type of naive Bayes, "beta", "logitnorm", "cauchy", "laplace", "gamma", "normlog" or "weibull". For the last 4 distributions, the negative of the logarithm of the compositional data is applied first.

**Value**

Depending on the classifier a list including (the ni and est are common for all classifiers):

shape	A matrix with the shape parameters.
scale	A matrix with the scale parameters.
expmu	A matrix with the mean parameters.
sigma	A matrix with the (MLE, hence biased) variance parameters.
location	A matrix with the location parameters (medians).
scale	A matrix with the scale parameters.
mean	A matrix with the scale parameters.
var	A matrix with the variance parameters.
a	A matrix with the "alpha" parameters.

b	A matrix with the "beta" parameters.
ni	The sample size of each group in the dataset.
est	The estimated group of the xnew observations. It returns a numerical value back regardless of the target variable being numerical as well or factor. Hence, it is suggested that you do <code>as.numeric(ina)</code> in order to see what is the predicted class of the new data.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Friedman J., Hastie T. and Tibshirani R. (2017). The elements of statistical learning. New York: Springer.

**See Also**

[cv.compnb](#), [alfa.rda](#), [alfa.knn](#), [comp.knn](#), [mix.compnorm](#), [dda](#)

**Examples**

```
x <- Compositional::rdiri(100, runif(5) )
ina <- rbinom(100, 1, 0.5) + 1
a <- comp.nb(x, x, ina, type = "beta")
```

---

Naive Bayes classifiers for compositional data using the  
alpha-transformation

*Naive Bayes classifiers for compositional data using the  $\alpha$ -  
transformation*

---

**Description**

Naive Bayes classifiers for compositional data using the  $\alpha$ -transformation.

**Usage**

```
alfa.nb(xnew, x, ina, a, type = "gaussian")
```



**Arguments**

xnew	A matrix with the new compositional predictor data whose class you want to predict. Zeros are allowed.
x	A matrix with the available compositional predictor data. Zeros are allowed.
ina	A vector of data. The response variable, which is categorical (factor is acceptable).
a	This can be a vector of values or a single number.
type	The type of naive Bayes, "gaussian", "cauchy" or "laplace".

**Details**

The  $\alpha$ -transformation is applied to the compositional and a naive Bayes classifier is employed.

**Value**

A matrix with the estimated groups. One column for each value of  $\alpha$ .

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain. <https://arxiv.org/pdf/1106.1451.pdf>

Friedman J., Hastie T. and Tibshirani R. (2017). The elements of statistical learning. New York: Springer.

**See Also**

[comp.nb](#), [alfa.rda](#), [alfa.knn](#), [comp.knn](#), [mix.compnorm](#)

**Examples**

```
x <- Compositional::rdiri(100, runif(5) )
ina <- rbinom(100, 1, 0.5) + 1
mod <- alfa.nb(x, x, a = c(0, 0.1, 0.2), ina )
```

---

Non linear least squares regression for compositional data

*Non linear least squares regression for compositional data*

---

### Description

Non linear least squares regression for compositional data.

### Usage

```
ols.compreg(y, x, con = TRUE, B = 1, ncores = 1, xnew = NULL)
```

### Arguments

y	A matrix with the compositional data (dependent variable). Zero values are allowed.
x	A matrix or a data frame with the predictor variable(s).
con	If this is TRUE (default) then the constant term is estimated, otherwise the model includes no constant term.
B	If B is greater than 1 bootstrap estimates of the standard error are returned. If B=1, no standard errors are returned.
ncores	If ncores is 2 or more parallel computing is performed. This is to be used for the case of bootstrap. If B=1, this is not taken into consideration.
xnew	If you have new data use it, otherwise leave it NULL.

### Details

The ordinary least squares between the observed and the fitted compositional data is adopted as the objective function. This involves numerical optimization since the relationship is non linear. There is no log-likelihood.

### Value

A list including:

runtime	The time required by the regression.
beta	The beta coefficients.
covbe	The covariance matrix of the beta coefficients. If B=1, this is based on the observed information (Hessian matrix), otherwise if B> this is the bootstrap estimate.
est	The fitted of xnew if xnew is not NULL.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

## References

Murteira, Jose MR, and Joaquim JS Ramalho 2016. Regression analysis of multivariate fractional data. *Econometric Reviews* 35(4): 515-552.

## See Also

[diri.reg](#), [js.compreg](#), [kl.compreg](#), [comp.reg](#), [comp.reg](#), [alfa.reg](#)

## Examples

```
library(MASS)
x <- as.vector(fg1[, 1])
y <- as.matrix(fg1[, 2:9])
y <- y / rowSums(y)
mod1 <- ols.compreg(y, x, B = 1, ncores = 1)
mod2 <- js.compreg(y, x, B = 1, ncores = 1)
```

---

Non-parametric zero replacement strategies

*Non-parametric zero replacement strategies*

---

## Description

Non-parametric zero replacement strategies.

## Usage

```
zeroreplace(x, a = 0.65, delta = NULL, type = "multiplicative")
```

## Arguments

x	A matrix with the compositional data.
a	The replacement value ( $\delta$ ) will be "a" times the minimum value observed in the compositional data.
delta	Unless you specify the replacement value $\delta$ here.
type	This can be any of "multiplicative", "additive" or "simple". See the references for more details.

## Details

The "additive" is the zero replacement strategy suggested in Aitchison (1986, pg. 269). All of the three strategies can be found in Martin-Fernandez et al. (2003).

## Value

A matrix with the zero replaced compositional data.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Martin-Fernandez J. A., Barcelo-Vidal C. & Pawlowsky-Glahn, V. (2003). Dealing with zeros and missing values in compositional data sets using nonparametric imputation. *Mathematical Geology*, 35(3): 253-278.

Aitchison J. (1986). *The statistical analysis of compositional data*. Chapman & Hall.

**See Also**

[perturbation](#), [alfa](#)

**Examples**

```
x <- as.matrix(iris[1:20, 1:4])
x <- x / rowSums(x)
x[ sample(1:20, 4), sample(1:4, 1) ] <- 0
x <- x / rowSums(x)
zeroreplace(x)
```

---

Permutation linear independence test in the SCLS model

*Permutation linear independence test in the SCLS model*

---

**Description**

Permutation linear independence test in the SCLS model.

**Usage**

```
scls.indeptest(y, x, R = 999)
```

**Arguments**

y	A matrix with the compositional data (dependent variable). Zero values are allowed.
x	A matrix with the compositional predictors. Zero values are allowed.
R	The number of permutations to perform.

**Details**

Permutation independence test in the constrained linear least squares for compositional responses and predictors is performed. The observed test statistic is the MSE computed by [scls](#). Then, the rows of X are permuted B times and each time the constrained OLS is performed and the MSE is computed. The p-value is then computed in the usual way.

**Value**

The p-value for the test of independence between Y and X.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Tsagris. M. (2024). Constrained least squares simplicial-simplicial regression. <https://arxiv.org/pdf/2403.19835.pdf>

**See Also**

[scls](#), [scls2](#), [tflr](#), [scls.betest](#)

**Examples**

```
library(MASS)
set.seed(1234)
y <- rdiri(214, runif(4, 1, 3))
x <- as.matrix(fgl[, 2:9])
x <- x / rowSums(x)
scls.indeptest(y, x, R = 99)
```

---

Permutation linear independence test in the TFLR model

*Permutation linear independence test in the TFLR model*

---

**Description**

Permutation linear independence test in the TFLR model.

**Usage**

```
tflr.indeptest(y, x, R = 999, ncores = 1)
```

**Arguments**

y	A matrix with the compositional data (dependent variable). Zero values are allowed.
x	A matrix with the compositional predictors. Zero values are in general allowed, but there can be cases when these are problematic.
R	The number of permutations to perform.
ncores	The number of cores to use in case you are interested for parallel computations.

**Details**

Permutation independence test in the constrained linear least squares for compositional responses and predictors is performed. The observed test statistic is the Kullback-Leibler divergence computed by `tflr`. Then, the rows of  $X$  are permuted  $B$  times and each time the TFLR is performed and the Kullback-Leibler is computed. The p-value is then computed in the usual way.

**Value**

The p-value for the test of linear independence between the simplicial response  $Y$  and the simplicial predictor  $X$ .

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

**References**

Fiksel J., Zeger S. and Datta A. (2022). A transformation-free linear regression for compositional outcomes and predictors. *Biometrics*, 78(3): 974–987.

Tsagris. M. (2024). Constrained least squares simplicial-simplicial regression. <https://arxiv.org/pdf/2403.19835.pdf>

**See Also**

`tflr`, `scls`, `tflr.betest`

**Examples**

```
library(MASS)
set.seed(1234)
y <- rdiri(214, runif(4, 1, 3))
x <- as.matrix(fgl[, 2:9])
x <- x / rowSums(x)
tflr.indeptest(y, x, R = 9)
```

---

Permutation test for the matrix of coefficients in the SCLS model

*Permutation test for the matrix of coefficients in the SCLS model*

---

**Description**

Permutation test for the matrix of coefficients in the SCLS model.

**Usage**

```
scls.betest(y, x, B, R = 999)
```

**Arguments**

y	A matrix with the compositional data (dependent variable). Zero values are allowed.
x	A matrix with the compositional predictors. Zero values are allowed.
B	A specific matrix of coefficients to test. Under the null hypothesis, the matrix of coefficients is equal to this matrix.
R	The number of permutations to perform.

**Details**

Permutation independence test in the constrained linear least squares for compositional responses and predictors is performed. The observed test statistic is the MSE computed by [scls](#). Then, the rows of X are permuted B times and each time the constrained OLS is performed and the MSE is computed. The p-value is then computed in the usual way.

**Value**

The p-value for the test of independence between Y and X.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

**References**

Tsagris, M. (2024). Constrained least squares simplicial-simplicial regression. <https://arxiv.org/pdf/2403.19835.pdf>

**See Also**

[scls](#), [scls2](#), [tflr](#), [scls.indeptest](#), [tflr.indeptest](#)

**Examples**

```
y <- rdiri(100, runif(3, 1, 3) )
x <- rdiri(100, runif(3, 1, 3) )
B <- diag(3)
scls.betest(y, x, B = B, R = 99)
```

---

Permutation test for the matrix of coefficients in the TFLR model  
*Permutation test for the matrix of coefficients in the TFLR model*

---

### Description

Permutation test for the matrix of coefficients in the TFLR model.

### Usage

```
tflr.betest(y, x, B, R = 999, ncores = 1)
```

### Arguments

y	A matrix with the compositional data (dependent variable). Zero values are allowed.
x	A matrix with the compositional predictors. Zero values are in general allowed, but there can be cases when these are problematic.
B	A specific matrix of coefficients to test. Under the null hypothesis, the matrix of coefficients is equal to this matrix.
R	The number of permutations to perform.
ncores	The number of cores to use in case you are interested for parallel computations.

### Details

Permutation independence test in the constrained linear least squares for compositional responses and predictors is performed. The observed test statistic is the Kullback-Leibler divergence computed by `tflr`. Then, the rows of X are permuted B times and each time the TFLR is performed and the Kullback-Leibler is computed. The p-value is then computed in the usual way.

### Value

The p-value for the test of linear independence between the simplicial response Y and the simplicial predictor X.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

### References

Fiksel J., Zeger S. and Datta A. (2022). A transformation-free linear regression for compositional outcomes and predictors. *Biometrics*, 78(3): 974–987.

Tsagris. M. (2024). Constrained least squares simplicial-simplicial regression. <https://arxiv.org/pdf/2403.19835.pdf>



**See Also**

[tflr](#), [tflr.indeptest](#), [scls](#), [scls.indeptest](#)

**Examples**

```
y <- rdiri(100, runif(3, 1, 3) )
x <- rdiri(100, runif(3, 1, 3) )
B <- diag(3)
tflr.betest(y, x, B = B, R = 99)
```

---

Perturbation operation

*Perturbation operation*

---

**Description**

Perturbation operation.

**Usage**

```
perturbation(x, y, oper = "+")
```

**Arguments**

x	A matrix with the compositional data.
y	Either a matrix with compositional data or a vector with compositional data. In either case, the data may not be compositional data, as long as they non negative.
oper	For the summation this must be "*" and for the negation it must be "/". According to Aitchison (1986), multiplication is equal to summation in the log-space, and division is equal to negation.

**Details**

This is the perturbation operation defined by Aitchison (1986).

**Value**

A matrix with the perturbed compositional data.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

**References**

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

**See Also**[power](#)**Examples**

```
x <- as.matrix(iris[1:15, 1:4])
y <- as.matrix(iris[21:35, 1:4])
perturbation(x, y)
perturbation(x, y[1, ])
```

---

Plot of the LASSO coefficients

*Plot of the LASSO coefficients*

---

**Description**

Plot of the LASSO coefficients.

**Usage**

```
lassocoeff.plot(lasso, lambda = TRUE)
```

**Arguments**

lasso	An object where you have saved the result of the LASSO regression. See the examples for more details.
lambda	If you want the x-axis to contain the logarithm of the penalty parameter $\log(\lambda)$ set this to TRUE. Otherwise the x-axis will contain the $L_1$ -norm of the coefficients.

**Details**

This function plots the  $L_2$ -norm of the coefficients of each predictor variable versus the  $\log(\lambda)$  or the  $L_1$ -norm of the coefficients. This is the same plot as the one produced by the glmnet package with `type.coef = "2norm"`.

**Value**

A plot of the  $L_2$ -norm of the coefficients of each predictor variable (y-axis) versus the  $L_1$ -norm of all the coefficients (x-axis).

**Author(s)**

Michail Tsagris and Abdulaziz Alenazi.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Abdulaziz Alenazi <a.alenazi@nbu.edu.sa>. <a.alenazi@nbu.edu.sa>.

## References

Alenazi, A. A. (2022). f-divergence regression models for compositional data. *Pakistan Journal of Statistics and Operation Research*, 18(4): 867–882.

Friedman, J., Hastie, T. and Tibshirani, R. (2010) Regularization Paths for Generalized Linear Models via Coordinate Descent. *Journal of Statistical Software*, Vol. 33(1), 1–22.

## See Also

[lasso.klcompreg](#), [cv.lasso.klcompreg](#), [lasso.compreg](#), [cv.lasso.compreg](#), [kl.compreg](#), [comp.reg](#)

## Examples

```
y <- as.matrix(iris[, 1:4])
y <- y / rowSums(y)
x <- matrix( rnorm(150 * 30), ncol = 30 )
a <- lasso.klcompreg(y, x)
lassocoeff.plot(a)
b <- lasso.compreg(y, x)
lassocoeff.plot(b)
```

---

Power operation

*Power operation*

---

## Description

Power operation.

## Usage

```
pow(x, a)
```

## Arguments

x	A matrix with the compositional data.
a	Either a vector with numbers of a single number.

## Details

This is the power operation defined by Aitchison (1986). It is also the starting point of the  $\alpha$ -transformation.

## Value

A matrix with the power transformed compositional data.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain. <http://arxiv.org/pdf/1106.1451.pdf>

**See Also**

[perturbation](#), [alfa](#)

**Examples**

```
x <- as.matrix(iris[1:15, 1:4])
a <- runif(1)
pow(x, a)
```

---

Principal component analysis

*Principal component analysis*

---

**Description**

Principal component analysis.

**Usage**

```
logpca(x, center = TRUE, scale = TRUE, k = NULL, vectors = FALSE)
```

**Arguments**

x	A matrix with the compositional data. Zero values are not allowed.
center	Do you want your data centered? TRUE or FALSE.
scale	Do you want each of your variables scaled, i.e. to have unit variance? TRUE or FALSE.
k	If you want a specific number of eigenvalues and eigenvectors set it here, otherwise all eigenvalues (and eigenvectors if requested) will be returned.
vectors	Do you want the eigenvectors be returned? By default this is FALSE.

**Details**

The logarithm is applied to the compositional data and PCA is performed.

**Value**

A list including:

values            The eigenvalues.  
vectors           The eigenvectors.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

**See Also**

[alfa.pca](#), [alfa.pcr](#), [kl.alfapcr](#)

**Examples**

```
x <- as.matrix(iris[, 1:4])
x <- x/ rowSums(x)
a <- logpca(x)
```

---

Principal component analysis using the alpha-transformation

*Principal component analysis using the  $\alpha$ -transformation*

---

**Description**

Principal component analysis using the  $\alpha$ -transformation.

**Usage**

```
alfa.pca(x, a, center = TRUE, scale = TRUE, k = NULL, vectors = FALSE)
```

**Arguments**

x                    A matrix with the compositional data. Zero values are allowed. In that case "a" should be positive.

a                    The value of  $\alpha$  to use in the  $\alpha$ -transformation.

center              Do you want your data centered? TRUE or FALSE.

scale                Do you want each of your variables scaled, i.e. to have unit variance? TRUE or FALSE.

k                    If you want a specific number of eigenvalues and eigenvectors set it here, otherwise all eigenvalues (and eigenvectors if requested) will be returned.

vectors             Do you want the eigenvectors be returned? By default this is FALSE.

**Details**

The  $\alpha$ -transformation is applied to the compositional data and then PCA is performed. Note however, that the right multiplication by the Helmert sub-matrix is not applied in order to be in accordance with Aitchison (1983). When  $\alpha = 0$ , this results to the PCA proposed by Aitchison (1983).

**Value**

A list including:

values	The eigenvalues.
vectors	The eigenvectors.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

Aitchison, J. (1983). Principal component analysis of compositional data. *Biometrika*, 70(1), 57-65.

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain. <http://arxiv.org/pdf/1106.1451.pdf>

**See Also**

[logpca](#), [alfa.pcr](#), [kl.alfapcr](#)

**Examples**

```
x <- as.matrix(iris[, 1:4])
x <- x/ rowSums(x)
a <- alfa.pca(x, 0.5)
```

---

Principal component generalised linear models

*Principal component generalised linear models*

---

**Description**

Principal component generalised linear models.

**Usage**

```
glm.pcr(y, x, k = 1, xnew = NULL)
```

**Arguments**

<code>y</code>	A numerical vector with 0 and 1 (binary) or a vector with discrete (count) data.
<code>x</code>	A matrix with the predictor variable(s), they have to be continuous.
<code>k</code>	A number greater than or equal to 1. How many principal components to use. You may get results for the sequence of principal components.
<code>xnew</code>	If you have new data use it, otherwise leave it NULL.

**Details**

Principal component regression is performed with binary logistic or Poisson regression, depending on the nature of the response variable. The principal components of the cross product of the independent variables are obtained and classical regression is performed. This is used in the function [alfa.pcr](#).

**Value**

A list including:

<code>model</code>	The summary of the logistic or Poisson regression model as returned by the package Rfast.
<code>per</code>	The percentage of variance of the predictor variables retained by the <code>k</code> principal components.
<code>vec</code>	The principal components, the loadings.
<code>est</code>	The fitted or the predicted values (if <code>xnew</code> is not NULL). If the argument <code>k</code> is a vector then this is a matrix with the estimated values for each number of components.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

**References**

Aguilera A.M., Escabias M. and Valderrama M.J. (2006). Using principal components for estimating logistic regression with high-dimensional multicollinear data. *Computational Statistics & Data Analysis* 50(8): 1905-1924.

Jolliffe I.T. (2002). *Principal Component Analysis*.

**See Also**

[alfa.pcr](#), [alfapcr.tune](#)

**Examples**

```
x <- as.matrix(iris[, 1:4])
y <- rbinom(150, 1, 0.6)
mod <- glm.pcr(y, x, k = 1)
```

---

Principal coordinate analysis using the alpha-distance  
*Principal coordinate analysis using the  $\alpha$ -distance*

---

**Description**

Principal coordinate analysis using the  $\alpha$ -distance.

**Usage**

```
alfa.mds(x, a, k = 2, eig = TRUE)
```

**Arguments**

x	A matrix with the compositional data. Zero values are allowed.
a	The value of a. In case of zero values in the data it has to be greater than 1.
k	The maximum dimension of the space which the data are to be represented in. This can be a number between 1 and $D - 1$ , where $D$ denotes the number of dimensions.
eig	Should eigenvalues be returned? The default value is TRUE.

**Details**

The function computes the  $\alpha$ -distance matrix and then plugs it into the classical multidimensional scaling function in the "cmdscale" function.

**Value**

A list with the results of "cmdscale" function.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

- Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.
- Cox, T. F. and Cox, M. A. A. (2001). Multidimensional Scaling. Second edition. Chapman and Hall.
- Mardia, K. V., Kent, J. T. and Bibby, J. M. (1979). Chapter 14 of Multivariate Analysis, London: Academic Press.
- Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain. <https://arxiv.org/pdf/1106.1451.pdf>



**See Also**

[esov.mds](#), [alfa.pca](#),

**Examples**

```
x <- as.matrix(iris[, 1:4])
x <- x/ rowSums(x)
a <- esov.mds(x)
```

---

Principal coordinate analysis using the Jensen-Shannon divergence

*Principal coordinate analysis using the Jensen-Shannon divergence*

---

**Description**

Principal coordinate analysis using the Jensen-Shannon divergence.

**Usage**

```
esov.mds(x, k = 2, eig = TRUE)
```

**Arguments**

x	A matrix with the compositional data. Zero values are allowed.
k	The maximum dimension of the space which the data are to be represented in. This can be a number between 1 and $D - 1$ , where $D$ denotes the number of dimensions.
eig	Should eigenvalues be returned? The default value is TRUE.

**Details**

The function computes the Jensen-Shannon divergence matrix and then plugs it into the classical multidimensional scaling function in the "cmdscale" function.

**Value**

A list with the results of "cmdscale" function.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

- Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.
- Cox, T. F. and Cox, M. A. A. (2001). Multidimensional Scaling. Second edition. Chapman and Hall.
- Mardia, K. V., Kent, J. T. and Bibby, J. M. (1979). Chapter 14 of Multivariate Analysis, London: Academic Press.
- Tsagris, Michail (2015). A novel, divergence based, regression for compositional data. Proceedings of the 28th Panhellenic Statistics Conference, 15-18/4/2015, Athens, Greece. <https://arxiv.org/pdf/1511.07600.pdf>

**See Also**

[alfa.mds](#), [alfa.pca](#),

**Examples**

```
x <- as.matrix(iris[, 1:4])
x <- x/ rowSums(x)
a <- esov.mds(x)
```

---

Projection pursuit regression for compositional data

*Projection pursuit regression for compositional data*

---

**Description**

Projection pursuit regression for compositional data.

**Usage**

```
comp.ppr(y, x, nterms = 3, type = "alr", xnew = NULL, yb = NULL )
```

**Arguments**

y	A matrix with the compositional data.
x	A matrix with the continuous predictor variables or a data frame including categorical predictor variables.
nterms	The number of terms to include in the final model.
type	Either "alr" or "ilr" corresponding to the additive or the isometric log-ratio transformation respectively.
xnew	If you have new data use it, otherwise leave it NULL.
yb	If you have already transformed the data using a log-ratio transformation put it here. Othewise leave it NULL.

**Details**

This is the standard projection pursuit. See the built-in function "ppr" for more details.

**Value**

A list including:

runtime	The runtime of the regression.
mod	The produced model as returned by the function "ppr".
est	The fitted values of xnew if xnew is not NULL.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Friedman, J. H. and Stuetzle, W. (1981). Projection pursuit regression. *Journal of the American Statistical Association*, 76, 817-823. doi: 10.2307/2287576.

**See Also**

[compppr.tune](#), [aknn.reg](#), [akern.reg](#), [comp.reg](#), [kl.compreg](#), [alfa.reg](#)

**Examples**

```
y <- as.matrix(iris[, 1:3])
y <- y/ rowSums(y)
x <- iris[, 4]
mod <- comp.ppr(y, x)
```

---

Projection pursuit regression with compositional predictor variables

*Projection pursuit regression with compositional predictor variables*

---

**Description**

Projection pursuit regression with compositional predictor variables.

**Usage**

```
pprcomp(y, x, nterms = 3, type = "log", xnew = NULL)
```

**Arguments**

y	A numerical vector with the continuous variable.
x	A matrix with the compositional data. No zero values are allowed.
nterms	The number of terms to include in the final model.
type	Either "alr" or "log" corresponding to the additive log-ratio transformation or the simple logarithm applied to the compositional data.
xnew	If you have new data use it, otherwise leave it NULL.

## Details

This is the standard projection pursuit. See the built-in function "ppr" for more details. When the data are transformed with the additive log-ratio transformation this is close in spirit to the log-contrast regression.

## Value

A list including:

runtime	The runtime of the regression.
mod	The produced model as returned by the function "ppr".
est	The fitted values of xnew if xnew is not NULL.

## Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

## References

Friedman, J. H. and Stuetzle, W. (1981). Projection pursuit regression. *Journal of the American Statistical Association*, 76, 817-823. doi: 10.2307/2287576.

## See Also

[pprcomp.tune](#), [ice.pprcomp](#), [alfa.pcr](#), [lc.reg](#), [comp.ppr](#)

## Examples

```
x <- as.matrix( iris[, 2:4] )
x <- x/ rowSums(x)
y <- iris[, 1]
pprcomp(y, x)
```

---

Projection pursuit regression with compositional predictor variables  
using the alpha-transformation

*Projection pursuit regression with compositional predictor variables  
using the  $\alpha$ -transformation*

---

## Description

Projection pursuit regression with compositional predictor variables using the  $\alpha$ -transformation.

## Usage

```
alfa.pprcomp(y, x, nterms = 3, a, xnew = NULL)
```

## Arguments

y	A numerical vector with the continuous variable.
x	A matrix with the compositional data. Zero values are allowed.
nterms	The number of terms to include in the final model.
a	The value of $\alpha$ for the $\alpha$ -transformation.
xnew	If you have new data use it, otherwise leave it NULL.

## Details

This is the standard projection pursuit. See the built-in function "ppr" for more details. The compositional data are transformed with the  $\alpha$ -transformation

## Value

A list including:

runtime	The runtime of the regression.
mod	The produced model as returned by the function "ppr".
est	The fitted values of xnew if xnew is not NULL.

## Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

## References

Friedman, J. H. and Stuetzle, W. (1981). Projection pursuit regression. *Journal of the American Statistical Association*, 76, 817-823. doi: 10.2307/2287576.

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In *Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain*. <https://arxiv.org/pdf/1106.1451.pdf>

## See Also

[alfapprcomp.tune](#), [pprcomp](#), [comp.ppr](#)

## Examples

```
x <- as.matrix( iris[, 2:4] )
x <- x / rowSums(x)
y <- iris[, 1]
alfa.pprcomp(y, x, a = 0.5)
```

---

Projections based test for distributional equality of two groups  
*Projections based test for distributional equality of two groups*

---

**Description**

Projections based test for distributional equality of two groups.

**Usage**

```
dptest(x1, x2, B = 100)
```

**Arguments**

x1	A matrix containing compositional data of the first group.
x2	A matrix containing compositional data of the second group.
B	The number of random uniform projections to use.

**Details**

The test compares the distributions of two compositional datasets using random projections. For more details see Cuesta-Albertos, Cuevas and Fraiman (2009).

**Value**

A vector including:

pvalues	The p-values of the Kolmogorov-Smirnov tests.
pvalue	The p-value of the test based on the Benjamini and Heller (2008) procedure.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Cuesta-Albertos J. A., Cuevas A. and Fraiman, R. (2009). On projection-based tests for directional and compositional data. *Statistics and Computing*, 19: 367–380.

Benjamini Y. and Heller R. (2008). Screening for partial conjunction hypotheses. *Biometrics*, 64(4): 1215–1222.

**See Also**

[comp.test](#)

**Examples**

```
x1 <- rdirich(50, c(3, 4, 5)) ## Fisher distribution with low concentration
x2 <- rdirich(50, c(3, 4, 5))
dptest(x1, x2)
```

---

Proportionality correlation coefficient matrix

*Proportionality correlation coefficient matrix*

---

**Description**

Proportionality correlation coefficient matrix.

**Usage**

```
pcc(x)
```

**Arguments**

`x` A numerical matrix with the compositional data. Zeros are not allowed as the logarithm is applied.

**Details**

The function returns the proportionality correlation coefficient matrix. See Lovell et al. (2015) for more information.

**Value**

A matrix with the alr transformed data (if alr is used) or with the compositional data (if the alrinv is used).

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Zheng, B. (2000). Summarizing the goodness of fit of generalized linear models for longitudinal data. *Statistics in medicine*, 19(10), 1265-1275.

Lovell D., Pawlowsky-Glahn V., Egozcue J. J., Marguerat S. and Bahler, J. (2015). Proportionality: a valid alternative to correlation for relative data. *PLoS Computational Biology*, 11(3), e1004075.

**See Also**

[acor](#), [alr](#)

**Examples**

```
x <- Compositional::rdiri(100, runif(4) )
a <- Compositional::pcc(x)
```

---

Quasi binomial regression for proportions

*Quasi binomial regression for proportions*

---

**Description**

Quasi binomial regression for proportions.

**Usage**

```
propreg(y, x, varb = "quasi", tol = 1e-07, maxiters = 100)
propregs(y, x, varb = "quasi", tol = 1e-07, logged = FALSE, maxiters = 100)
```

**Arguments**

y	A numerical vector proportions. 0s and 1s are allowed.
x	For the "propreg" a matrix with data, the predictor variables. This can be a matrix or a data frame. For the "propregs" this must be a numerical matrix, where each columns denotes a variable.
tol	The tolerance value to terminate the Newton-Raphson algorithm. This is set to $10^{-9}$ by default.
varb	The type of estimate to be used in order to estimate the covariance matrix of the regression coefficients. There are two options, either "quasi" (default value) or "glm". See the references for more information.
logged	Should the p-values be returned (FALSE) or their logarithm (TRUE)?
maxiters	The maximum number of iterations before the Newton-Raphson is terminated automatically.

**Details**

We are using the Newton-Raphson, but unlike R's built-in function "glm" we do no checks and no extra calculations, or whatever. Simply the model. The "propregs" is to be used for very many univariate regressions. The "x" is a matrix in this case and the significance of each variable (column of the matrix) is tested. The function accepts binary responses as well (0 or 1).

**Value**

For the "propreg" function a list including:

iters	The number of iterations required by the Newton-Raphson.
varb	The covariance matrix of the regression coefficients.



phi            The phi parameter is returned if the input argument "varb" was set to "glm", otherwise this is NULL.

info           A table similar to the one produced by "glm" with the estimated regression coefficients, their standard error, Wald test statistic and p-values.

For the "propregs" a two-column matrix with the test statistics (Wald statistic) and the associated p-values (or their loggarithm).

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

### References

Papke L. E. & Wooldridge J. (1996). Econometric methods for fractional response variables with an application to 401(K) plan participation rates. *Journal of Applied Econometrics*, 11(6): 619–632.

McCullagh, Peter, and John A. Nelder. *Generalized linear models*. CRC press, USA, 2nd edition, 1989.

### See Also

[ols.compreg beta.reg](#)

### Examples

```
y <- rbeta(100, 1, 4)
x <- matrix(rnorm(100 * 3), ncol = 3)
a <- propreg(y, x)
y <- rbeta(100, 1, 4)
x <- matrix(rnorm(400 * 100), ncol = 400)
b <- propregs(y, x)
mean(b[, 2] < 0.05)
```

---

Random values generation from some univariate distributions defined on the (0,1) interval

*Random values generation from some univariate distributions defined on the (0,1) interval*

---

### Description

Random values generation from some univariate distributions defined on the (0,1) interval.

### Usage

```
rbeta1(n, a)
runitweibull(n, a, b)
rlogitnorm(n, m, s, fast = FALSE)
```

**Arguments**

<code>n</code>	The sample size, a numerical value.
<code>a</code>	The shape parameter of the beta distribution. In the case of the unit Weibull, this is the shape parameter.
<code>b</code>	This is the scale parameter for the unit Weibull distribution.
<code>m</code>	The mean of the univariate normal in $R$ .
<code>s</code>	The standard deviation of the univariate normal in $R$ .
<code>fast</code>	If you want a faster generation set this equal to TRUE. This will use the <code>Rnorm()</code> function from the <code>Rfast</code> package. However, the speed is only observable if you want to simulate at least 500 (this number may vary among computers) observations. The larger the sample size the higher the speed-up.

**Details**

The function generates random values from the  $Be(a, 1)$ , the unit Weibull or the univariate logistic normal distribution.

**Value**

A vector with the simulated data.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**See Also**

[beta.est](#), [colbeta.est](#), [rdiri](#)

**Examples**

```
x <- rbeta1(100, 3)
```

---

Read a file as a Filebacked Big Matrix

*Read a file as a Filebacked Big Matrix*

---

**Description**

Read a file as a Filebacked Big Matrix.

**Usage**

```
read.fbm(file, select)
```

**Arguments**

file	The File to read.
select	Indices of columns to read (sorted). The length of select will be the number of columns of the resulting FBM.

**Details**

The functions read a file as a Filebacked Big Matrix object. For more information see the "bigstatsr" package.

**Value**

A Filebacked Big Matrix object.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**See Also**

[scls](#)

**Examples**

```
x <- matrix( runif(50 * 20, 0, 2*pi), ncol = 20 )
```

---

Regression with compositional data using the alpha-transformation

*Regression with compositional data using the  $\alpha$ -transformation*

---

**Description**

Regression with compositional data using the  $\alpha$ -transformation.

**Usage**

```
alfa.reg(y, x, a, xnew = NULL, yb = NULL)  
alfa.reg2(y, x, a, xnew = NULL)  
alfa.reg3(y, x, a = c(-1, 1), xnew = NULL)
```

**Arguments**

<code>y</code>	A matrix with the compositional data.
<code>x</code>	A matrix with the continuous predictor variables or a data frame including categorical predictor variables.
<code>a</code>	The value of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ the isometric log-ratio transformation is applied and the solution exists in a closed form, since it the classical multivariate regression. For the <code>alfa.reg2()</code> this should be a vector of $\alpha$ values and the function call repeatedly the <code>alfa.reg()</code> function. For the <code>alfa.reg3()</code> function it should be a vector with two values, the endpoints of the interval of $\alpha$ . This function searches for the optimal value of $\alpha$ that minimizes the sum of squares of the errors. Using the <code>optimize</code> function it searches for the optimal value of $\alpha$ . Instead of choosing the value of $\alpha$ using <code>alfareg.tune</code> (that uses cross-validation) one can select it this way.
<code>xnew</code>	If you have new data use it, otherwise leave it NULL.
<code>yb</code>	If you have already transformed the data using the $\alpha$ -transformation with the same $\alpha$ as given in the argument "a", put it here. Otherwise leave it NULL. This is intended to be used in the function <code>alfareg.tune</code> in order to speed up the process. The time difference in that function is small for small samples. But, if you have a few thousands and or a few more components, there will be bigger differences.

**Details**

The  $\alpha$ -transformation is applied to the compositional data first and then multivariate regression is applied. This involves numerical optimisation. The `alfa.reg2()` function accepts a vector with many values of  $\alpha$ , while the `alfa.reg3()` function searches for the value of  $\alpha$  that minimizes the Kulback-Leibler divergence between the observed and the fitted compositional values. The functions are highly optimized.

**Value**

For the `alfa.reg()` function a list including:

<code>runtime</code>	The time required by the regression.
<code>be</code>	The beta coefficients.
<code>seb</code>	The standard error of the beta coefficients.
<code>est</code>	The fitted values for <code>xnew</code> if <code>xnew</code> is not NULL.

For the `alfa.reg2()` function a list with as many sublists as the number of values of  $\alpha$ . Each element (sublist) of the list contains the above outcomes of the `alfa.reg()` function.

For the `alfa.reg3()` function a list with all previous elements plus an output "alfa", the optimal value of  $\alpha$ .

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

## References

- Tsagris M. (2015). Regression analysis with compositional data containing zero values. *Chilean Journal of Statistics*, 6(2): 47-57. <https://arxiv.org/pdf/1508.01913v1.pdf>
- Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In *Proceedings of the 4th Compositional Data Analysis Workshop*, Girona, Spain. <https://arxiv.org/pdf/1106.1451.pdf>
- Mardia K.V., Kent J.T., and Bibby J.M. (1979). *Multivariate analysis*. Academic press.
- Aitchison J. (1986). *The statistical analysis of compositional data*. Chapman & Hall.

## See Also

[alfareg.tune](#), [diri.reg](#), [js.compreg](#), [kl.compreg](#), [ols.compreg](#), [comp.reg](#)

## Examples

```
library(MASS)
x <- as.vector(fgl[1:40, 1])
y <- as.matrix(fgl[1:40, 2:9])
y <- y / rowSums(y)
mod <- alfa.reg(y, x, 0.2)
```

---

Regularised and flexible discriminant analysis for compositional data using the alpha-transformation

*Regularised and flexible discriminant analysis for compositional data using the  $\alpha$ -transformation*

---

## Description

Regularised and flexible discriminant analysis for compositional data using the  $\alpha$ -transformation.

## Usage

```
alfa.rda(xnew, x, ina, a, gam = 1, del = 0)
alfa.fda(xnew, x, ina, a)
```

## Arguments

- |      |  |
|------|--|
| xnew | A matrix with the new compositional data whose group is to be predicted. Zeros are allowed, but you must be careful to choose strictly positive values of $\alpha$ . |
| x    | A matrix with the available compositional data. Zeros are allowed, but you must be careful to choose strictly positive values of $\alpha$ .                          |
| ina  | A group indicator variable for the available data.   |
| a    | The value of $\alpha$ for the $\alpha$ -transformation.  |
| gam  | This is a number between 0 and 1. It is the weight of the pooled covariance and the diagonal matrix.   |
| del  | This is a number between 0 and 1. It is the weight of the LDA and QDA.   |

## Details

For the `alfa.rda`, the covariance matrix of each group is calculated and then the pooled covariance matrix. The spherical covariance matrix consists of the average of the pooled variances in its diagonal and zeros in the off-diagonal elements. `gam` is the weight of the pooled covariance matrix and `1-gam` is the weight of the spherical covariance matrix,  $S_a = \text{gam} * S_p + (1-\text{gam}) * s_p$ . Then it is a compromise between LDA and QDA. `del` is the weight of  $S_a$  and `1-del` the weight of each group covariance group.

For the `alfa.fda` a flexible discriminant analysis is performed. See the R package **fda** for more details.

## Value

For the `alfa.rda` a list including:

<code>prob</code>	The estimated probabilities of the new data of belonging to each group.
<code>scores</code>	The estimated scores of the new data of each group.
<code>est</code>	The estimated group membership of the new data.

For the `alfa.fda` a list including:

<code>mod</code>	An <code>fda</code> object as returned by the command <code>fda</code> of the R package <code>mda</code> .
<code>est</code>	The estimated group membership of the new data.

## Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)> and Giorgos Athineou <[gioathineou@gmail.com](mailto:gioathineou@gmail.com)>.

## References

Friedman Jerome, Trevor Hastie and Robert Tibshirani (2009). *The elements of statistical learning*, 2nd edition. Springer, Berlin.

Tsagris Michail, Simon Preston and Andrew T.A. Wood (2016). Improved classification for compositional data using the  $\alpha$ -transformation. *Journal of classification*, 33(2): 243-261. <https://arxiv.org/pdf/1106.1451.pdf>

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In *Proceedings of the 4th Compositional Data Analysis Workshop*, Girona, Spain. <https://arxiv.org/pdf/1106.1451.pdf>

Hastie, Tibshirani and Buja (1994). Flexible Discriminant Analysis by Optimal Scoring. *Journal of the American Statistical Association*, 89(428):1255-1270.

## See Also

[alfa](#), [alfarda.tune](#), [alfa.knn](#), [alfa.nb](#), [comp.nb](#), [mix.compnorm](#)

**Examples**

```
x <- as.matrix(iris[, 1:4])
x <- x / rowSums(x)
ina <- iris[, 5]
mod <- alfa.rda(x, x, ina, 0)
table(ina, mod$est)
mod2 <- alfa.fda(x, x, ina, 0)
table(ina, mod2$est)
```

---

Regularised discriminant analysis for Euclidean data

*Regularised discriminant analysis for Euclidean data*

---

**Description**

Regularised discriminant analysis for Euclidean data.

**Usage**

```
rda(xnew, x, ina, gam = 1, del = 0)
```

**Arguments**

xnew	A matrix with the new data whose group is to be predicted. They have to be continuous.
x	A matrix with the available data. They have to be continuous.
ina	A group indicator variable for the available data.
gam	This is a number between 0 and 1. It is the weight of the pooled covariance and the diagonal matrix.
del	This is a number between 0 and 1. It is the weight of the LDA and QDA.

**Details**

The covariance matrix of each group is calculated and then the pooled covariance matrix. The spherical covariance matrix consists of the average of the pooled variances in its diagonal and zeros in the off-diagonal elements.  $\text{gam}$  is the weight of the pooled covariance matrix and  $1-\text{gam}$  is the weight of the spherical covariance matrix,  $S_a = \text{gam} * S_p + (1-\text{gam}) * s_p$ . Then it is a compromise between LDA and QDA.  $\text{del}$  is the weight of  $S_a$  and  $1-\text{del}$  the weight of each group covariance group.

**Value**

A list including:

prob	The estimated probabilities of the new data of belonging to each group.
scores	The estimated scores of the new data of each group.
est	The estimated group membership of the new data.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Friedman J.H. (1989): Regularized Discriminant Analysis. *Journal of the American Statistical Association* 84(405): 165–175.

Friedman Jerome, Trevor Hastie and Robert Tibshirani (2009). *The elements of statistical learning*, 2nd edition. Springer, Berlin.

Tsagris M., Preston S. and Wood A.T.A. (2016). Improved classification for compositional data using the  $\alpha$ -transformation. *Journal of Classification*, 33(2): 243–261.

**See Also**

[rda.tune](#)

**Examples**

```
x <- as.matrix(iris[, 1:4])
ina <- iris[, 5]
mod <- rda(x, x, ina)
table(ina, mod$est)
```

---

Ridge regression

*Ridge regression*

---

**Description**

Ridge regression.

**Usage**

```
ridge.reg(y, x, lambda, B = 1, xnew = NULL)
```

**Arguments**

y	A real valued vector. If it contains percentages, the logit transformation is applied.
x	A matrix with the predictor variable(s), they have to be continuous.
lambda	The value of the regularisation parameter $\lambda$ .
B	If B = 1 (default value) no bootstrpa is performed. Otherwise bootstrap standard errors are returned.
xnew	If you have new data whose response value you want to predict put it here, otherwise leave it as is.



**Details**

This is used in the function `alfa.ridge`. There is also a built-in function available from the MASS library, called "lm.ridge".

**Value**

A list including:

<code>beta</code>	The beta coefficients.
<code>seb</code>	The standard error of the coefficients. If $B > 1$ the bootstrap standard errors will be returned.
<code>est</code>	The fitted or the predicted values (if <code>xnew</code> is not NULL).

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Giorgos Athineou <gioathineou@gmail.com>.

**References**

Hoerl A.E. and R.W. Kennard (1970). Ridge regression: Biased estimation for nonorthogonal problems. *Technometrics*, 12(1): 55-67.

Brown P. J. (1994). *Measurement, Regression and Calibration*. Oxford Science Publications.

**See Also**

[ridge.tune](#), [alfa.ridge](#), [ridge.plot](#)

**Examples**

```
y <- as.vector(iris[, 1])
x <- as.matrix(iris[, 2:4])
mod1 <- ridge.reg(y, x, lambda = 0.1)
mod2 <- ridge.reg(y, x, lambda = 0)
```

---

Ridge regression plot *Ridge regression plot*

---

**Description**

A plot of the regularised regression coefficients is shown.

**Usage**

```
ridge.plot(y, x, lambda = seq(0, 5, by = 0.1) )
```

**Arguments**

y	A numeric vector containing the values of the target variable. If the values are proportions or percentages, i.e. strictly within 0 and 1 they are mapped into R using the logit transformation. In any case, they must be continuous only.
x	A numeric matrix containing the continuous variables. Rows are samples and columns are features.
lambda	A grid of values of the regularisation parameter $\lambda$ .

**Details**

For every value of  $\lambda$  the coefficients are obtained. They are plotted versus the  $\lambda$  values.

**Value**

A plot with the values of the coefficients as a function of  $\lambda$ .

**Author(s)**

Michail Tsagris.

R implementation and documentation: Giorgos Athineou <gioathineou@gmail.com> and Michail Tsagris <mtsagris@uoc.gr>.

**References**

Hoerl A.E. and R.W. Kennard (1970). Ridge regression: Biased estimation for nonorthogonal problems. *Technometrics*, 12(1): 55-67.

Brown P. J. (1994). *Measurement, Regression and Calibration*. Oxford Science Publications.

**See Also**

[ridge.reg](#), [ridge.tune](#), [alfa.ridge](#), [alfaridge.plot](#)

**Examples**

```
y <- as.vector(iris[, 1])
x <- as.matrix(iris[, 2:4])
ridge.plot(y, x, lambda = seq(0, 2, by = 0.1) )
```

Ridge regression with compositional data in the covariates side using the alpha-transformation

*Ridge regression with compositional data in the covariates side using the  $\alpha$ -transformation*

---

## Description

Ridge regression with compositional data in the covariates side using the  $\alpha$ -transformation.

## Usage

```
alfa.ridge(y, x, a, lambda, B = 1, xnew = NULL)
```

## Arguments

y	A numerical vector containing the response variable values. If they are percentages, they are mapped onto $R$ using the logit transformation.
x	A matrix with the predictor variables, the compositional data. Zero values are allowed, but you must be careful to choose strictly positive values of $\alpha$ .
a	The value of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ the isometric log-ratio transformation is applied.
lambda	The value of the regularisation parameter, $\lambda$ .
B	If $B > 1$ bootstrap estimation of the standard errors is implemented.
xnew	A matrix containing the new compositional data whose response is to be predicted. If you have no new data, leave this NULL as is by default.

## Details

The  $\alpha$ -transformation is applied to the compositional data first and then ridge components regression is performed.

## Value

The output of the [ridge.reg](#).

## Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Giorgos Athineou <gioathineou@gmail.com>.

**References**

Tsagris M. (2015). Regression analysis with compositional data containing zero values. *Chilean Journal of Statistics*, 6(2): 47-57. <https://arxiv.org/pdf/1508.01913v1.pdf>

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In *Proceedings of the 4th Compositional Data Analysis Workshop*, Girona, Spain. <https://arxiv.org/pdf/1106.1451.pdf>

**See Also**

[ridge.reg](#), [alfaridge.tune](#), [alfaridge.plot](#)

**Examples**

```
library(MASS)
y <- as.vector(fgl[, 1])
x <- as.matrix(fgl[, 2:9])
x <- x/ rowSums(x)
mod1 <- alfa.ridge(y, x, a = 0.5, lambda = 0.1, B = 1, xnew = NULL)
mod2 <- alfa.ridge(y, x, a = 0.5, lambda = 1, B = 1, xnew = NULL)
```

---

Ridge regression with the alpha-transformation plot  
*Ridge regression plot*

---

**Description**

A plot of the regularised regression coefficients is shown.

**Usage**

```
alfaridge.plot(y, x, a, lambda = seq(0, 5, by = 0.1) )
```

**Arguments**

y	A numeric vector containing the values of the target variable. If the values are proportions or percentages, i.e. strictly within 0 and 1 they are mapped into R using the logit transformation. In any case, they must be continuous only.
x	A numeric matrix containing the continuous variables.
a	The value of the $\alpha$ -transformation. It has to be between -1 and 1. If there are zero values in the data, you must use a strictly positive value.
lambda	A grid of values of the regularisation parameter $\lambda$ .

**Details**

For every value of  $\lambda$  the coefficients are obtained. They are plotted versus the  $\lambda$  values.

**Value**

A plot with the values of the coefficients as a function of  $\lambda$ .

**Author(s)**

Michail Tsagris.

R implementation and documentation: Giorgos Athineou <gioathineou@gmail.com> and Michail Tsagris <mtsagris@uoc.gr>.

**References**

Hoerl A.E. and R.W. Kennard (1970). Ridge regression: Biased estimation for nonorthogonal problems. *Technometrics*, 12(1): 55-67.

Brown P. J. (1994). *Measurement, Regression and Calibration*. Oxford Science Publications.

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In *Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain*. <https://arxiv.org/pdf/1106.1451.pdf>

**See Also**

[ridge.plot](#), [alfa.ridge](#)

**Examples**

```
library(MASS)
y <- as.vector(fgl[, 1])
x <- as.matrix(fgl[, 2:9])
x <- x / rowSums(x)
alfaridge.plot(y, x, a = 0.5, lambda = seq(0, 5, by = 0.1) )
```

---

Simplicial constrained median regression for compositional responses  
and predictors model

*Simplicial constrained median regression for compositional responses  
and predictors*

---

**Description**

Simplicial constrained median regression for compositional responses and predictors.

**Usage**

```
scrq(y, x, xnew = NULL)
```

**Arguments**

y	A matrix with the compositional data (dependent variable). Zero values are allowed.
x	A matrix with the compositional predictors. Zero values are allowed.
xnew	If you have new data use it, otherwise leave it NULL.

**Details**

The function performs median regression where the beta coefficients are constrained to be positive and sum to 1.

**Value**

A list including:

mlad	The mean absolute deviation.
be	The beta coefficients.
est	The fitted of xnew if xnew is not NULL.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Tsagris, M. (2024). Constrained least squares simplicial-simplicial regression. <https://arxiv.org/pdf/2403.19835.pdf>

**See Also**

[scls](#), [tflr](#)

**Examples**

```
library(MASS)
set.seed(1234)
y <- rdiri(214, runif(4, 1, 3))
x <- as.matrix(fgl[, 2:9])
x <- x / rowSums(x)
mod <- scrq(y, x)
mod
```

---

Simulation of compositional data from Gaussian mixture models

*Simulation of compositional data from Gaussian mixture models*

---

## Description

Simulation of compositional data from Gaussian mixture models.

## Usage

```
rmixcomp(n, prob, mu, sigma, type = "alr")
```

## Arguments

n	The sample size.
prob	A vector with mixing probabilities. Its length is equal to the number of clusters.
mu	A matrix where each row corresponds to the mean vector of each cluster.
sigma	An array consisting of the covariance matrix of each cluster.
type	Should the additive ("type=alr") or the isometric (type="ilr") log-ratio be used? The default value is for the additive log-ratio transformation.

## Details

A sample from a multivariate Gaussian mixture model is generated.

## Value

A list including:

id	A numeric variable indicating the cluster of simulated vector.
x	A matrix containing the simulated compositional data. The number of dimensions will be + 1.

## Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

## References

Ryan P. Browne, Aisha ElSherbiny and Paul D. McNicholas (2015). R package mixture: Mixture Models for Clustering and Classification.

## See Also

[mix.compnorm](#), [bic.mixcompnorm](#)

**Examples**

```
p <- c(1/3, 1/3, 1/3)
mu <- matrix(nrow = 3, ncol = 4)
s <- array( dim = c(4, 4, 3) )
x <- as.matrix(iris[, 1:4])
ina <- as.numeric(iris[, 5])
mu <- rowsum(x, ina) / 50
s[, , 1] <- cov(x[ina == 1, ])
s[, , 2] <- cov(x[ina == 2, ])
s[, , 3] <- cov(x[ina == 3, ])
y <- rmixcomp(100, p, mu, s, type = "alr")
```

---

Simulation of compositional data from mixtures of Dirichlet distributions

*Simulation of compositional data from mixtures of Dirichlet distributions*

---

**Description**

Simulation of compositional data from mixtures of Dirichlet distributions.

**Usage**

```
rmixdiri(n, a, prob)
```

**Arguments**

n	The sample size.
a	A matrix where each row contains the parameters of each Dirichlet component.
prob	A vector with the mixing probabilities.

**Details**

A sample from a Dirichlet mixture model is generated.

**Value**

A list including:

id	A numeric variable indicating the cluster of simulated vector.
x	A matrix containing the simulated compositional data.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.



## References

Ye X., Yu Y. K. and Altschul S. F. (2011). On the inference of Dirichlet mixture priors for protein sequence comparison. *Journal of Computational Biology*, 18(8), 941-954.

## See Also

[rmixcomp](#), [mixdiri.contour](#),

## Examples

```
a <- matrix( c(12, 30, 45, 32, 50, 16), byrow = TRUE, ncol = 3)
prob <- c(0.5, 0.5)
x <- rmixdiri(100, a, prob)
```

---

Simulation of compositional data from the Flexible Dirichlet distribution

*Simulation of compositional data from the Flexible Dirichlet distribution*

---

## Description

Simulation of compositional data from the Flexible Dirichlet distribution.

## Usage

```
rfd(n, alpha, prob, tau)
```

## Arguments

n	The sample size.
alpha	A vector of the non-negative $\alpha$ parameters.
prob	A vector of the clusters' probabilities that must sum to one.
tau	The positive scalar $\tau$ parameter.

## Details

For more information see the references and the package `FlxeDir`.

## Value

A matrix with compositional data.

## Author(s)

Michail Tsagris ported from the R package `FlexDir`. <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

**References**

Ongaro A. and Migliorati S. (2013). A generalization of the Dirichlet distribution. *Journal of Multivariate Analysis*, 114, 412–426.

Migliorati S., Ongaro A. and Monti G. S. (2017). A structured Dirichlet mixture model for compositional data: inferential and applicative issues. *Statistics and Computing*, 27, 963–983.

**See Also**

[dfd](#)

**Examples**

```
alpha <- c(12, 11, 10)
prob <- c(0.25, 0.25, 0.5)
x <- rfd(100, alpha, prob, 7)
```

---

Simulation of compositional data from the folded normal distribution  
*Simulation of compositional data from the folded model normal distribution*

---

**Description**

Simulation of compositional data from the folded model normal distribution.

**Usage**

```
rfolded(n, mu, su, a)
```

**Arguments**

n	The sample size.
mu	The mean vector.
su	The covariance matrix.
a	The value of $\alpha$ .

**Details**

A sample from the folded model is generated.

**Value**

A matrix with compositional data.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Tsagris M. and Stewart C. (2020). A folded model for compositional data analysis. Australian and New Zealand Journal of Statistics, 62(2): 249-277. <https://arxiv.org/pdf/1802.07330.pdf>

**See Also**

[alfa](#), [alpha.mle](#), [a.est](#)

**Examples**

```
s <- c(0.1490676523, -0.4580818209, 0.0020395316, -0.0047446076, -0.4580818209,
1.5227259250, 0.0002596411, 0.0074836251, 0.0020395316, 0.0002596411,
0.0365384838, -0.0471448849, -0.0047446076, 0.0074836251, -0.0471448849,
0.0611442781)
s <- matrix(s, ncol = 4)
m <- c(1.715, 0.914, 0.115, 0.167)
x <- rfolded(100, m, s, 0.5)
a.est(x)
```

---

Spatial median regression

*Spatial median regression*

---

**Description**

Spatial median regression with Euclidean data.

**Usage**

```
spatmed.reg(y, x, xnew = NULL, tol = 1e-07, ses = FALSE)
```

**Arguments**

y	A matrix with the compositional data. Zero values are not allowed.
x	The predictor variable(s), they have to be continuous.
xnew	If you have new data use it, otherwise leave it NULL.
tol	The threshold upon which to stop the iterations of the Newton-Rapshon algorithm.
ses	If you want to extract the standard errors of the parameters, set this to TRUE. Be careful though as this can slow down the algorithm dramatically. In a run example with 10,000 observations and 10 variables for y and 30 for x, when ses = FALSE the algorithm can take 0.20 seconds, but when ses = TRUE it can go up to 140 seconds.

**Details**

The objective function is the minimization of the sum of the absolute residuals. It is the multivariate generalization of the median regression. This function is used by [comp.reg](#).

**Value**

A list including:

<code>iter</code>	The number of iterations that were required.
<code>runtime</code>	The time required by the regression.
<code>be</code>	The beta coefficients.
<code>seb</code>	The standard error of the beta coefficients is returned if <code>ses=TRUE</code> and <code>NULL</code> otherwise.
<code>est</code>	The fitted of <code>xnew</code> if <code>xnew</code> is not <code>NULL</code> .

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

**References**

Biman Chakraborty (2003). On multivariate quantile regression. *Journal of Statistical Planning and Inference*, 110(1-2), 109-132. [http://www.stat.nus.edu.sg/export/sites/dsap/research/documents/tr01\\_2000.pdf](http://www.stat.nus.edu.sg/export/sites/dsap/research/documents/tr01_2000.pdf)

**See Also**

[multivreg](#), [comp.reg](#), [alfa.reg](#), [js.compreg](#), [diri.reg](#)

**Examples**

```
library(MASS)
x <- as.matrix(iris[, 3:4])
y <- as.matrix(iris[, 1:2])
mod1 <- spatmed.reg(y, x)
mod2 <- multivreg(y, x, plot = FALSE)
```

---

Ternary diagram

*Ternary diagram*

---

**Description**

Ternary diagram.

**Usage**

```
ternary(x, dg = FALSE, hg = FALSE, means = TRUE, pca = FALSE, colour = NULL)
```

**Arguments**

x	A matrix with the compositional data.
dg	Do you want diagonal grid lines to appear? If yes, set this TRUE.
hg	Do you want horizontal grid lines to appear? If yes, set this TRUE.
means	A boolean variable. Should the closed geometric mean and the arithmetic mean appear (TRUE) or not (FALSE)?.
pca	Should the first PCA calculated Aitchison (1983) described appear? If yes, then this should be TRUE, or FALSE otherwise.
colour	If you want the points to appear in different colour put a vector with the colour numbers or colours.

**Details**

There are two ways to create a ternary graph. We used here that one where each edge is equal to 1 and it is what Aitchison (1986) uses. For every given point, the sum of the distances from the edges is equal to 1. Horizontal and or diagonal grid lines can appear, so as the closed geometric and the simple arithmetic mean. The first PCA is calculated using the centred log-ratio transformation as Aitchison (1983, 1986) suggested. If the data contain zero values, the first PCA will not be plotted. Zeros in the data appear with green circles in the triangle and you will also see NaN in the closed geometric mean.

**Value**

The ternary plot and a 2-row matrix with the means. The closed geometric and the simple arithmetic mean vector and or the first principal component will appear as well if the user has asked for them. Additionally, horizontal or diagonal grid lines can appear as well.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Giorgos Athineou <gioathineou@gmail.com>.

**References**

- Aitchison, J. (1983). Principal component analysis of compositional data. *Biometrika* 70(1):57-65.  
Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

**See Also**

[ternary.mcr](#), [ternary.reg](#), [diri.contour](#)

**Examples**

```
x <- as.matrix(iris[, 1:3])
x <- x / rowSums(x)
ternary(x, means = TRUE, pca = TRUE)
```

---

Ternary diagram of regression models

*Ternary diagram of regression models*

---

### Description

Ternary diagram of regression models.

### Usage

```
ternary.reg(y, est, id, labs)
```

### Arguments

<code>y</code>	A matrix with the compositional data.
<code>est</code>	A matrix with all fitted compositional data for all regression models, one under the other.
<code>id</code>	A vector indicating the regression model of each fitted compositional data set.
<code>labs</code>	The names of the regression models to appear in the legend.

### Details

The points first appear on the ternary plot. Then, the fitted compositional data appear with different lines for each regression model.

### Value

The ternary plot and lines for the fitted values of each regression model.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

### References

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

### See Also

[ternary](#), [ternary.mcr](#), [diri.contour](#)

*Ternary diagram with confidence region for the matrix of coefficients of the SCLS or the TFLR model*<sup>199</sup>

### Examples

```
x <- cbind(1, rnorm(50) )
a <- exp( x %%% matrix( rnorm(6,0, 0.4), ncol = 3) )
y <- matrix(NA, 50, 3)
for (i in 1:50) y[i, ] <- rdiri(1, a[i, ])
est <- comp.reg(y, x[, -1], xnew = x[, -1])$est
ternary.reg(y, est, id = rep(1, 50), labs = "ALR regression")
```

---

Ternary diagram with confidence region for the matrix of coefficients  
of the SCLS or the TFLR model

*Ternary diagram with confidence region for the matrix of coefficients  
of the SCLS or the TFLR model*

---

### Description

Ternary diagram with confidence region for the matrix of coefficients of the SCLS or the TFLR model.

### Usage

```
ternary.coefcr(y, x, type = "scls", conf = 0.95, R = 1000, dg = FALSE, hg = FALSE)
```

### Arguments

y	A matrix with the response compositional data.
x	A matrix with the predictor compositional data.
type	The type of model to use, "scls" or "tflr". Depending on the model selected, the function will construct the confidence regions of the estimated matrix of coefficients of that model.
conf	The confidence level, by default this is set to 0.95.
R	Number of bootstrap replicates to run.
dg	Do you want diagonal grid lines to appear? If yes, set this TRUE.
hg	Do you want horizontal grid lines to appear? If yes, set this TRUE.

### Details

This function runs the SCLS or the TFLR model and constructs confidence regions for the estimated matrix of regression coefficients using non-parametric bootstrap.

### Value

A ternary plot of the estimated matrix of coefficients of the SCLS or of the TFLR model, and their associated confidence regions.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Fiksel J., Zeger S. and Datta A. (2022). A transformation-free linear regression for compositional outcomes and predictors. *Biometrics*, 78(3): 974–987.

Tsagris. M. (2024). Constrained least squares simplicial-simplicial regression. <https://arxiv.org/pdf/2403.19835.pdf>

**See Also**

[ternary](#), [scls](#), [tflr](#), [ternary.mcr](#)

**Examples**

```
y <- rdiri(50, runif(3))
x <- rdiri(50, runif(4))
ternary.coefcr(y, x, R = 500, dg = TRUE, hg = TRUE)
```

---

Ternary diagram with confidence region for the mean

*Ternary diagram with confidence region for the mean*

---

**Description**

Ternary diagram with confidence region for the mean.

**Usage**

```
ternary.mcr(x, type = "alr", conf = 0.95, dg = FALSE, hg = FALSE, colour = NULL)
```

**Arguments**

x	A matrix with the compositional data.
dg	Do you want diagonal grid lines to appear? If yes, set this TRUE.
type	The type of log-ratio transformation to apply, the "alr" or the "ilr".
conf	The confidence level, by default this is set to 0.95.
hg	Do you want horizontal grid lines to appear? If yes, set this TRUE.
colour	If you want the points to appear in different colour put a vector with the colour numbers or colours.

**Details**

Ternary plot of compositional data including the log-ratio mean and its confidence region. The confidence region is based on the Hotelling  $T^2$  test statistic of the log-ratio transformed data.



**Value**

A ternary plot of compositional data including the log-ratio mean and its confidence region.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Aitchison, J. (1983). Principal component analysis of compositional data. *Biometrika* 70(1):57-65.

Aitchison J. (1986). *The statistical analysis of compositional data*. Chapman & Hall.

**See Also**

[ternary](#), [ternary.reg](#), [diri.contour](#)

**Examples**

```
x <- as.matrix(iris[, 1:3])
x <- x / rowSums(x)
ternary.mcr(x, type = "alr", dg = TRUE, hg = TRUE)
```

---

Ternary diagram with the coefficients of the simplicial-simplicial regression models

*Ternary diagram with the coefficients of the simplicial-simplicial regression models*

---

**Description**

Ternary diagram with the coefficients of the simplicial-simplicial regression models.

**Usage**

```
ternary.coef(B, dg = FALSE, hg = FALSE, colour = NULL)
```

**Arguments**

B	A matrix with the coefficients of the <a href="#">tflr</a> or the <a href="#">scls</a> functions. See examples for this.
dg	Do you want diagonal grid lines to appear? If yes, set this TRUE.
hg	Do you want horizontal grid lines to appear? If yes, set this TRUE.
colour	If you want the points to appear in different colour put a vector with the colour numbers or colours.

**Details**

Ternary plot of the coefficients of the `tflr` or the `scls` functions.

**Value**

A ternary plot of the coefficients of the `tflr` or the `scls` functions.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Aitchison, J. (1983). Principal component analysis of compositional data. *Biometrika* 70(1):57-65.

Aitchison J. (1986). *The statistical analysis of compositional data*. Chapman & Hall.

**See Also**

[ternary](#), [ternary.reg](#), [scls](#)

**Examples**

```
y <- as.matrix(iris[, 1:3])
y <- y / rowSums(y)
x <- rdir(150, runif(5, 1,4) )
mod <- scls(y, x)
ternary.coef(mod$be)
```

---

The additive log-ratio transformation and its inverse

*The additive log-ratio transformation and its inverse*

---

**Description**

The additive log-ratio transformation and its inverse.

**Usage**

```
alr(x)
alrinv(y)
```

**Arguments**

`x` A numerical matrix with the compositional data.  
`y` A numerical matrix with data to be closed into the simplex.

**Details**

The additive log-ratio transformation with the first component being the common divisor is applied. The inverse of this transformation is also available. This means that no zeros are allowed.

**Value**

A matrix with the alr transformed data (if alr is used) or with the compositional data (if the alrinv is used).

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

**See Also**

[bc](#), [pivot](#), [fp](#), [green](#), [alfa](#), [alfainv](#)

**Examples**

```
library(MASS)
x <- as.matrix(fg1[, 2:9])
x <- x / rowSums(x)
y <- alr(x)
x1 <- alrinv(y)
```

---

The alpha-distance      *The  $\alpha$ -distance*

---

**Description**

This is the Euclidean (or Manhattan) distance after the  $\alpha$ -transformation has been applied.

**Usage**

```
alfadist(x, a, type = "euclidean", square = FALSE)
alfadista(xnew, x, a, type = "euclidean", square = FALSE)
```

**Arguments**

xnew	A matrix or a vector with new compositional data.
x	A matrix with the compositional data.
a	The value of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ , the isometric log-ratio transformation is applied.
type	Which type distance do you want to calculate after the $\alpha$ -transformation, "euclidean", or "manhattan".
square	In the case of the Euclidean distance, you can choose to return the squared distance by setting this TRUE.

**Details**

The  $\alpha$ -transformation is applied to the compositional data first and then the Euclidean or the Manhattan distance is calculated.

**Value**

For "alfadist" a matrix including the pairwise distances of all observations or the distances between xnew and x. For "alfadista" a matrix including the pairwise distances of all observations or the distances between xnew and x.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Tsagris M.T., Preston S. and Wood A.T.A. (2016). Improved classification for compositional data using the  $\alpha$ -transformation. *Journal of Classification*. 33(2): 243–261. <https://arxiv.org/pdf/1506.04976v2.pdf>

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In *Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain*. <https://arxiv.org/pdf/1106.1451.pdf>

**See Also**

[alfa](#), [alfainv](#), [alfa.reg](#), [esov](#)

**Examples**

```
library(MASS)
x <- as.matrix(fgl[1:20, 2:9])
x <- x / rowSums(x)
alfadist(x, 0.1)
alfadist(x, 1)
```

---

The alpha-IT transformation  
*The  $\alpha$ -IT transformation*

---

**Description**

The  $\alpha$ -IT transformation.

**Usage**

```
ait(x, a, h = TRUE)
```

**Arguments**

x	A matrix with the compositional data.
a	The value of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ the isometric log-ratio transformation is applied.
h	A boolean variable. If is TRUE (default value) the multiplication with the Helmert sub-matrix will take place. When $\alpha = 0$ and h = FALSE, the result is the centred log-ratio transformation (Aitchison, 1986). In general, when h = FALSE the resulting transformation maps the data onto a singular space. The sum of the vectors is equal to 0. Hence, from the simplex constraint the data go to another constraint.

**Details**

The  $\alpha$ -IT transformation is applied to the compositional data.

**Value**

A matrix with the  $\alpha$ -IT transformed data.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Clarotto L., Allard D. and Menafoglio A. (2022). A new class of  $\alpha$ -transformations for the spatial analysis of Compositional Data. *Spatial Statistics*, 47.

**See Also**

[aitdist](#), [ait.knn](#), [alfa](#), [green](#), [alr](#)

**Examples**

```
library(MASS)
x <- as.matrix(fgl[, 2:9])
x <- x / rowSums(x)
y1 <- ait(x, 0.2)
y2 <- ait(x, 1)
rbind( colMeans(y1), colMeans(y2) )
```

---

The alpha-IT-distance *The  $\alpha$ -IT-distance*

---

**Description**

This is the Euclidean (or Manhattan) distance after the  $\alpha$ -IT-transformation has been applied.

**Usage**

```
aitdist(x, a, type = "euclidean", square = FALSE)
aitdista(xnew, x, a, type = "euclidean", square = FALSE)
```

**Arguments**

xnew	A matrix or a vector with new compositional data.
x	A matrix with the compositional data.
a	The value of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ , the isometric log-ratio transformation is applied.
type	Which type distance do you want to calculate after the $\alpha$ -transformation, "euclidean", or "manhattan".
square	In the case of the Euclidean distance, you can choose to return the squared distance by setting this TRUE.

**Details**

The  $\alpha$ -IT-transformation is applied to the compositional data first and then the Euclidean or the Manhattan distance is calculated.

**Value**

For "alfadist" a matrix including the pairwise distances of all observations or the distances between xnew and x. For "alfadista" a matrix including the pairwise distances of all observations or the distances between xnew and x.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Clarotto L., Allard D. and Menafoglio A. (2021). A new class of  $\alpha$ -transformations for the spatial analysis of Compositional Data. <https://arxiv.org/abs/2110.07967>

**See Also**

[ait](#), [alfadist](#), [alfa](#)

**Examples**

```
library(MASS)
x <- as.matrix(fgl[1:20, 2:9])
x <- x / rowSums(x)
aitdist(x, 0.1)
aitdist(x, 1)
```

---

The alpha-k-NN regression for compositional response data

*The  $\alpha$ -k-NN regression for compositional response data*

---

**Description**

The  $\alpha$ -k-NN regression for compositional response data.

**Usage**

```
aknn.reg(xnew, y, x, a = seq(0.1, 1, by = 0.1), k = 2:10,
apostasi = "euclidean", rann = FALSE)
```

**Arguments**

xnew	A matrix with the new predictor variables whose compositions are to be predicted.
y	A matrix with the compositional response data. Zeros are allowed.
x	A matrix with the available predictor variables.
a	The value(s) of $\alpha$ . Either a single value or a vector of values. As zero values in the compositional data are allowed, you must be careful to choose strictly positive values of $\alpha$ . However, if negative values are passed, the positive ones are used only.
k	The number of nearest neighbours to consider. It can be a single number or a vector.

<code>apostasi</code>	The type of distance to use, either "euclidean" or "manhattan".
<code>rann</code>	If you have large scale datasets and want a faster k-NN search, you can use kd-trees implemented in the R package "Rnanoflann". In this case you must set this argument equal to TRUE. Note however, that in this case, the only available distance is by default "euclidean".

### Details

The  $\alpha$ -k-NN regression for compositional response variables is applied.

### Value

A list with the estimated compositional response data for each value of  $\alpha$  and k.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

### References

Tsagris M., Alenazi A. and Stewart C. (2023). Flexible non-parametric regression models for compositional response data with zeros. *Statistics and Computing*, 33(106).

<https://link.springer.com/article/10.1007/s11222-023-10277-5>

### See Also

[aknnreg.tune](#), [akern.reg](#), [alfa.reg](#), [comp.ppr](#), [comp.reg](#), [kl.compreg](#)

### Examples

```
y <- as.matrix( iris[, 1:3] )
y <- y / rowSums(y)
x <- iris[, 4]
mod <- aknn.reg(x, y, x, a = c(0.4, 0.5), k = 2:3, apostasi = "euclidean")
```

---

The  $\alpha$ -k-NN regression with compositional predictor variables

*The  $\alpha$ -k-NN regression with compositional predictor variables*

---

### Description

The  $\alpha$ -k-NN regression with compositional predictor variables.

### Usage

```
alfa.knn.reg(xnew, y, x, a = 1, k = 2:10, apostasi = "euclidean", method = "average")
```



**Arguments**

xnew	A matrix with the new compositional predictor variables whose response is to be predicted. Zeros are allowed.
y	The response variable, a numerical vector.
x	A matrix with the available compositional predictor variables. Zeros are allowed.
a	A single value of $\alpha$ . As zero values in the compositional data are allowed, you must be careful to choose strictly positive values of $\alpha$ . If negative values are passed, the positive ones are used only. If the data are already alpha-transformed, you can make this NULL.
k	The number of nearest neighbours to consider. It can be a single number or a vector.
apostasi	The type of distance to use, either "euclidean" or "manhattan".
method	If you want to take the average of the responses of the k closest observations, type "average". For the median, type "median" and for the harmonic mean, type "harmonic".

**Details**

The  $\alpha$ -k-NN regression with compositional predictor variables is applied.

**Value**

A matrix with the estimated response data for each value of k.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Tsagris M., Alenazi A. and Stewart C. (2023). Flexible non-parametric regression models for compositional response data with zeros. *Statistics and Computing*, 33(106).

<https://link.springer.com/article/10.1007/s11222-023-10277-5>

**See Also**

[aknn.reg](#), [alfa.knn](#), [alfa.pcr](#), [alfa.ridge](#)

**Examples**

```
library(MASS)
x <- as.matrix(fg1[, 2:9])
x <- x / rowSums(x)
y <- fg1[, 1]
mod <- alfa.knn.reg(x, y, x, a = 0.5, k = 2:4)
```

---

The alpha-kernel regression with compositional response data

*The  $\alpha$ -kernel regression with compositional response data*

---

### Description

The  $\alpha$ -kernel regression with compositional response data.

### Usage

```
akern.reg( xnew, y, x, a = seq(0.1, 1, by = 0.1),
h = seq(0.1, 1, length = 10), type = "gauss" )
```

### Arguments

xnew	A matrix with the new predictor variables whose compositions are to be predicted.
y	A matrix with the compositional response data. Zeros are allowed.
x	A matrix with the available predictor variables.
a	The value(s) of $\alpha$ . Either a single value or a vector of values. As zero values in the compositional data are allowed, you must be careful to choose strictly positive values of $\alpha$ . However, if negative values are passed, the positive ones are used only.
h	The bandwidth value(s) to consider.
type	The type of kernel to use, "gauss" or "laplace".

### Details

The  $\alpha$ -kernel regression for compositional response variables is applied.

### Value

A list with the estimated compositional response data for each value of  $\alpha$  and h.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

### References

Tsagris M., Alenazi A. and Stewart C. (2023). Flexible non-parametric regression models for compositional response data with zeros. *Statistics and Computing*, 33(106).

<https://link.springer.com/article/10.1007/s11222-023-10277-5>

**See Also**

[akernreg.tune](#), [aknn.reg](#), [aknnreg.tune](#), [alfa.reg](#), [comp.ppr](#), [comp.reg](#), [kl.compreg](#)

**Examples**

```
y <- as.matrix( iris[, 1:3] )
y <- y / rowSums(y)
x <- iris[, 4]
mod <- akern.reg( x, y, x, a = c(0.4, 0.5), h = c(0.1, 0.2) )
```

---

The alpha-SCLS model    *The  $\alpha$ -SCLS model for compositional responses and predictors*

---

**Description**

The  $\alpha$ -SCLS model for compositional responses and predictors.

**Usage**

```
ascls(y, x, a = seq(0.1, 1, by = 0.1), xnew)
```

**Arguments**

<code>y</code>	A matrix with the compositional data (dependent variable). Zero values are allowed.
<code>x</code>	A matrix with the compositional predictors. Zero values are allowed.
<code>a</code>	A vector or a single number of values of the $\alpha$ -parameter. This has to be different from zero, and it can take negative values if there are no zeros in the simplicial response ( <code>y</code> ).
<code>xnew</code>	The new data for which predictions will be made.

**Details**

This is an extension of the SCLS model that includes the  $\alpha$ -transformation and is intended solely for prediction purposes.

**Value**

A list with matrices containing the predicted simplicial response values, one matrix for each value of  $\alpha$ .

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

## References

Tsagris, M. (2024). Constrained least squares simplicial-simplicial regression. <https://arxiv.org/pdf/2403.19835.pdf>

## See Also

[scls](#), [cv.ascls](#), [atflr](#)

## Examples

```
library(MASS)
set.seed(1234)
y <- rdirichlet(214, runif(4, 1, 3))
x <- as.matrix(fgl[, 2:9])
x <- x / rowSums(x)
mod <- ascls(y, x, xnew = x)
mod
```

---

The alpha-TFLR model *The  $\alpha$ -TFLR model for compositional responses and predictors*

---

## Description

The  $\alpha$ -TFLR model for compositional responses and predictors.

## Usage

```
atflr(y, x, a = seq(0.1, 1, by = 0.1), xnew)
```

## Arguments

<code>y</code>	A matrix with the compositional data (dependent variable). Zero values are allowed.
<code>x</code>	A matrix with the compositional predictors. Zero values are allowed.
<code>a</code>	A vector or a single number of values of the $\alpha$ -parameter. This has to be different from zero, and it can take negative values if there are no zeros in the simplicial response ( <code>y</code> ).
<code>xnew</code>	The new data for which predictions will be made.

## Details

This is an extension of the TFLR model that includes the  $\alpha$ -transformation and is intended solely for prediction purposes.

## Value

A list with matrices containing the predicted simplicial response values, one matrix for each value of  $\alpha$ .

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Fiksel J., Zeger S. and Datta A. (2022). A transformation-free linear regression for compositional outcomes and predictors. *Biometrics*, 78(3): 974–987.

Tsagris. M. (2024). Constrained least squares simplicial-simplicial regression. <https://arxiv.org/pdf/2403.19835.pdf>

**See Also**

[tflr](#), [cv.atflr](#), [ascls](#)

**Examples**

```
library(MASS)
set.seed(1234)
y <- rdirich(214, runif(4, 1, 3))
x <- as.matrix(fgl[, 2:9])
x <- x / rowSums(x)
mod <- ascls(y, x, a = c(0.5, 1), xnew = x)
mod
```

---

The alpha-transformation

*The  $\alpha$ -transformation*

---

**Description**

The  $\alpha$ -transformation.

**Usage**

```
alfa(x, a, h = TRUE)
alef(x, a)
```

**Arguments**

**x** A matrix with the compositional data.

**a** The value of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If  $\alpha = 0$  the isometric log-ratio transformation is applied.

**h** A boolean variable. If is TRUE (default value) the multiplication with the Helmert sub-matrix will take place. When  $\alpha = 0$  and `h = FALSE`, the result is the centred log-ratio transformation (Aitchison, 1986). In general, when `h = FALSE` the resulting transformation maps the data onto a singular space. The sum of the vectors is equal to 0. Hence, from the simplex constraint the data go to another constraint.

### Details

The  $\alpha$ -transformation is applied to the compositional data. The command "`alef`" is the same as "`alfa(x, a, h = FALSE)`", but returns a different element as well and is necessary for the functions `a.est`, `a.mle` and `alpha.mle`.

### Value

A list including:

**sa** The logarithm of the Jacobian determinant of the  $\alpha$ -transformation. This is used in the "`profile`" function to speed up the computations.

**sk** If the "`alef`" was called, this will return the sum of the  $\alpha$ -power transformed data, prior to being normalised to sum to 1. If  $\alpha = 0$ , this will not be returned.

**aff** The  $\alpha$ -transformed data.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)> and Giorgos Athineou <[gioathineou@gmail.com](mailto:gioathineou@gmail.com)>.

### References

- Tsagris M. and Stewart C. (2022). A Review of Flexible Transformations for Modeling Compositional Data. In *Advances and Innovations in Statistics and Data Science*, pp. 225–234. [https://link.springer.com/chapter/10.1007/978-3-031-08329-7\\_10](https://link.springer.com/chapter/10.1007/978-3-031-08329-7_10)
- Tsagris Michail and Stewart Connie (2020). A folded model for compositional data analysis. *Australian and New Zealand Journal of Statistics*, 62(2): 249-277. <https://arxiv.org/pdf/1802.07330.pdf>
- Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In *Proceedings of the 4th Compositional Data Analysis Workshop*, Girona, Spain. <https://arxiv.org/pdf/1106.1451.pdf>
- Aitchison J. (1986). *The statistical analysis of compositional data*. Chapman & Hall.

### See Also

`alfainv`, `pivot`, `alfa.profile`, `alfa.tune`, `a.est`, `alpha.mle`, `alr`, `bc`, `fp`, `green`

**Examples**

```
library(MASS)
x <- as.matrix(fgl[, 2:9])
x <- x / rowSums(x)
y1 <- alfa(x, 0.2)$aff
y2 <- alfa(x, 1)$aff
rbind( colMeans(y1), colMeans(y2) )
y3 <- alfa(x, 0.2)$aff
dim(y1) ; dim(y3)
rowSums(y1)
rowSums(y3)
```

---

The Box-Cox transformation applied to ratios of components

*The Box-Cox transformation applied to ratios of components*

---

**Description**

The Box-Cox transformation applied to ratios of components.

**Usage**

```
bc(x, lambda)
```

**Arguments**

x	A matrix with the compositional data. The first component must be zero values free.
lambda	The value of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\lambda = 0$ the additive log-ratio transformation ( <a href="#">alr</a> ) is applied.

**Details**

The Box-Cox transformation applied to ratios of components, as described in Aitchison (1986) is applied.

**Value**

A matrix with the transformed data.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

**See Also**

[alr](#), [fp](#), [green](#), [alfa](#)

**Examples**

```
library(MASS)
x <- as.matrix(fgl[, 2:9])
x <- x / rowSums(x)
y1 <- bc(x, 0.2)
y2 <- bc(x, 0)
rbind( colMeans(y1), colMeans(y2) )
rowSums(y1)
rowSums(y2)
```

---

The ESOV-distance

*The ESOV-distance*

---

**Description**

The ESOV-distance.

**Usage**

```
esov(x)
esova(xnew, x)
es(x1, x2)
```

**Arguments**

x	A matrix with compositional data.
xnew	A matrix or a vector with new compositional data.
x1	A vector with compositional data.
x2	A vector with compositional data.

**Details**

The ESOV distance is calculated.

**Value**

For "esov()" a matrix including the pairwise distances of all observations or the distances between xnew and x.

For "esova()" a matrix including the pairwise distances of all observations or the distances between xnew and x.

For "es()" a number, the ESOV distance between x1 and x2.



**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Tsagris, Michail (2014). The k-NN algorithm for compositional data: a revised approach with and without zero values present. *Journal of Data Science*, 12(3): 519-534.

Endres, D. M. and Schindelin, J. E. (2003). A new metric for probability distributions. *Information Theory, IEEE Transactions on* 49, 1858-1860.

Osterreicher, F. and Vajda, I. (2003). A new class of metric divergences on probability spaces and its applicability in statistics. *Annals of the Institute of Statistical Mathematics* 55, 639-653.

**See Also**

[alfadist](#), [comp.knn](#), [js.compreg](#)

**Examples**

```
library(MASS)
x <- as.matrix(fg1[1:20, 2:9])
x <- x / rowSums(x)
esov(x)
```

---

The folded power transformation

*The folded power transformation*

---

**Description**

The folded power transformation.

**Usage**

```
fp(x, lambda)
```

**Arguments**

x	A matrix with the compositional data. Zero values are allowed.
lambda	The value of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\lambda = 0$ the additive log-ratio transformation ( <a href="#">alr</a> ) is applied. If zero values are present $\lambda$ must be strictly positive.

**Details**

The folded power transformation is applied to the compositional data.

**Value**

A matrix with the transformed data.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Atkinson, A. C. (1985). Plots, transformations and regression; an introduction to graphical methods of diagnostic regression analysis Oxford University Press.

**See Also**

[alr](#), [bc](#), [green](#), [alfa](#)

**Examples**

```
library(MASS)
x <- as.matrix(fg1[, 2:9])
x <- x / rowSums(x)
y1 <- fp(x, 0.2)
y2 <- fp(x, 0)
rbind( colMeans(y1), colMeans(y2) )
rowSums(y1)
rowSums(y2)
```

---

The Frechet mean for compositional data

*The Frechet mean for compositional data*

---

**Description**

Mean vector or matrix with mean vectors of compositional data using the  $\alpha$ -transformation.

**Usage**

```
frechet(x, a)
```

**Arguments**

**x** A matrix with the compositional data.

**a** The value of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If  $\alpha = 0$  the isometric log-ratio transformation is applied and the closed geometric mean is calculated. You can also provide a sequence of values of alpha and in this case a matrix of Frechet means will be returned.

**Details**

The power transformation is applied to the compositional data and the mean vector is calculated. Then the inverse of it is calculated and the inverse of the power transformation applied to the last vector is the Frechet mean.

**Value**

If  $\alpha$  is a single value, the function will return a vector with the Frechet mean for the given value of  $\alpha$ . Otherwise the function will return a matrix with the Frechet means for each value of  $\alpha$ .

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Giorgos Athineou <gioathineou@gmail.com>.

**References**

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain. <https://arxiv.org/pdf/1106.1451.pdf>

**See Also**

[alfa](#), [alfainv](#), [profile](#)

**Examples**

```
library(MASS)
x <- as.matrix(fg1[, 2:9])
x <- x / rowSums(x)
frechet(x, 0.2)
frechet(x, 1)
```

---

The Helmert sub-matrix

*The Helmert sub-matrix*

---

**Description**

The Helmert sub-matrix.

**Usage**

```
helm(n)
```

**Arguments**

`n` A number greater than or equal to 2.

**Details**

The Helmert sub-matrix is returned. It is an orthogonal matrix without the first row.

**Value**

A  $(n - 1) \times n$  matrix.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Giorgos Athineou <gioathineou@gmail.com>.

**References**

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain. <https://arxiv.org/pdf/1106.1451.pdf>

John Aitchison (2003). The Statistical Analysis of Compositional Data, p. 99. Blackburn Press.

Lancaster H. O. (1965). The Helmert matrices. The American Mathematical Monthly 72(1): 4-12.

**See Also**

[alfa](#), [alfainv](#)

**Examples**

```
helm(3)
helm(5)
```

---

The  $k$ -nearest neighbours using the alpha-distance

*The  $k$ -nearest neighbours using the  $\alpha$ -distance*

---

**Description**

The  $k$ -nearest neighbours using the  $\alpha$ -distance.

**Usage**

```
alfann(xnew, x, a, k = 10, rann = FALSE)
```

**Arguments**

xnew	A matrix or a vector with new compositional data.
x	A matrix with the compositional data.
a	The value of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ , the isometric log-ratio transformation is applied.
k	The number of nearest neighbours to search for.
rann	If you have large scale datasets and want a faster $k$ -NN search, you can use kd-trees implemented in the R package "Rnanoflann". In this case you must set this argument equal to TRUE. Note however, that in this case, the only available distance is by default "euclidean".

**Details**

The  $\alpha$ -transformation is applied to the compositional data first and the indices of the  $k$ -nearest neighbours using the Euclidean distance are returned.

**Value**

A matrix including the indices of the nearest neighbours of each xnew from x.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

MTsagris M., Alenazi A. and Stewart C. (2023). Flexible non-parametric regression models for compositional response data with zeros. *Statistics and Computing*, 33(106).

<https://link.springer.com/article/10.1007/s11222-023-10277-5>

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In *Proceedings of the 4th Compositional Data Analysis Workshop*, Girona, Spain.

<https://arxiv.org/pdf/1106.1451.pdf>

**See Also**

[alfa.knn](#), [comp.nb](#), [alfa.rda](#), [alfa.nb](#), [link{aknn.reg}](#), [alfa](#), [alfainv](#)

**Examples**

```
library(MASS)
xnew <- as.matrix(fgl[1:20, 2:9])
xnew <- xnew / rowSums(xnew)
x <- as.matrix(fgl[-c(1:20), 2:9])
x <- x / rowSums(x)
b <- alfann(xnew, x, a = 0.1, k = 10)
```

---

The k-NN algorithm for compositional data

*The k-NN algorithm for compositional data*

---

## Description

The k-NN algorithm for compositional data with and without using the power transformation.

## Usage

```
comp.knn(xnew, x, ina, a = 1, k = 5, apostasi = "ESOV", mesos = TRUE)
```

```
alfa.knn(xnew, x, ina, a = 1, k = 5, mesos = TRUE,
apostasi = "euclidean", rann = FALSE)
```

```
ait.knn(xnew, x, ina, a = 1, k = 5, mesos = TRUE,
apostasi = "euclidean", rann = FALSE)
```

## Arguments

xnew	A matrix with the new compositional data whose group is to be predicted. Zeros are allowed, but you must be careful to choose strictly positive values of $\alpha$ or not to set <code>apostasi = "Ait"</code> .
x	A matrix with the available compositional data. Zeros are allowed, but you must be careful to choose strictly positive values of $\alpha$ or not to set <code>apostasi = "Ait"</code> .
ina	A group indicator variable for the available data.
a	The value of $\alpha$ . As zero values in the compositional data are allowed, you must be careful to choose strictly positive values of $\alpha$ . You have the option to put <code>a = NULL</code> . In this case, the <code>xnew</code> and <code>x</code> are assumed to be the already $\alpha$ -transformed data.
k	The number of nearest neighbours to consider. It can be a single number or a vector.
apostasi	The type of distance to use. For the <code>comp.knn</code> this can be one of the following: "ESOV", "taxicab", "Ait", "Hellinger", "angular" or "CS". See the references for them. For the <code>alfa.knn</code> this can be either "euclidean" or "manhattan".
mesos	This is used in the non standard algorithm. If TRUE, the arithmetic mean of the distances is calculated, otherwise the harmonic mean is used (see details).
rann	If you have large scale datasets and want a faster k-NN search, you can use kd-trees implemented in the R package "Rnanoflann". In this case you must set this argument equal to TRUE. Note however, that in this case, the only available distance is by default "euclidean".

## Details

The k-NN algorithm is applied for the compositional data. There are many metrics and possibilities to choose from. The algorithm finds the k nearest observations to a new observation and allocates it to the class which appears most times in the neighbours. It then computes the arithmetic or the harmonic mean of the distances. The new point is allocated to the class with the minimum distance.

## Value

A vector with the estimated groups.

## Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Giorgos Athineou <gioathineou@gmail.com>.

## References

Tsagris, Michail (2014). The k-NN algorithm for compositional data: a revised approach with and without zero values present. *Journal of Data Science*, 12(3): 519–534.

Friedman Jerome, Trevor Hastie and Robert Tibshirani (2009). *The elements of statistical learning*, 2nd edition. Springer, Berlin

Tsagris Michail, Simon Preston and Andrew T.A. Wood (2016). Improved classification for compositional data using the  $\alpha$ -transformation. *Journal of Classification* 33(2): 243–261.

Connie Stewart (2017). An approach to measure distance between compositional diet estimates containing essential zeros. *Journal of Applied Statistics* 44(7): 1137–1152.

Clarotto L., Allard D. and Menafoglio A. (2022). A new class of  $\alpha$ -transformations for the spatial analysis of Compositional Data. *Spatial Statistics*, 47.

Endres, D. M. and Schindelin, J. E. (2003). A new metric for probability distributions. *Information Theory, IEEE Transactions on* 49, 1858–1860.

Osterreicher, F. and Vajda, I. (2003). A new class of metric divergences on probability spaces and its applicability in statistics. *Annals of the Institute of Statistical Mathematics* 55, 639–653.

## See Also

[compknn.tune](#), [alfa.rda](#), [comp.nb](#), [alfa.nb](#), [alfa.esov](#), [mix.compnorm](#)

## Examples

```
x <- as.matrix( iris[, 1:4] )
x <- x/ rowSums(x)
ina <- iris[, 5]
mod <- comp.knn(x, x, ina, a = 1, k = 5)
table(ina, mod)
mod2 <- alfa.knn(x, x, ina, a = 1, k = 5)
table(ina, mod2)
```

---

The multiplicative log-ratio transformation and its inverse

*The multiplicative log-ratio transformation and its inverse*

---

### Description

The multiplicative log-ratio transformation and its inverse.

### Usage

```
mlr(x)
mlrinv(y)
```

### Arguments

x                    A numerical matrix with the compositional data.  
y                    A numerical matrix with data to be closed into the simplex.

### Details

The multiplicative log-ratio transformation and its inverse are applied here. This means that no zeros are allowed.

### Value

A matrix with the mlr transformed data (if mlr is used) or with the compositional data (if the mlrinv is used).

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

### References

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

### See Also

[alr](#), [pivot](#), [green](#), [alfa](#)

### Examples

```
library(MASS)
x <- as.matrix(fg1[, 2:9])
x <- x / rowSums(x)
y <- mlr(x)
x1 <- mlrinv(y)
```



---

The pivot coordinate transformation and its inverse  
*The pivot coordinate transformation and its inverse*

---

**Description**

The pivot coordinate transformation and its inverse.

**Usage**

```
pivot(x)
pivotinv(y)
```

**Arguments**

x	A numerical matrix with the compositional data.
y	A numerical matrix with data to be closed into the simplex.

**Details**

The pivot coordinate transformation and its inverse are computed. This means that no zeros are allowed.

**Value**

A matrix with the alr transformed data (if pivot is used) or with the compositional data (if the pivotinv is used).

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Peter Filzmoser, Karel Hron and Matthias Templ (2018). Applied Compositional Data Analysis With Worked Examples in R (pages 49 and 51). Springer.

**See Also**

[alfa](#), [alfainv](#), [alr](#), [green](#)

**Examples**

```
library(MASS)
x <- as.matrix(fgl[, 2:9])
x <- x / rowSums(x)
y <- pivot(x)
x1 <- alrinv(y)
```

---

The SCLS model	<i>Simplicial constrained linear least squares (SCLS) for compositional responses and predictors</i>
----------------	--

---

### Description

Simplicial constrained linear least squares (SCLS) for compositional responses and predictors.

### Usage

```
scls(y, x, xnew = NULL, nbcores = 4)
```

### Arguments

y	A matrix with the compositional data (dependent variable). Zero values are allowed. It may also be a big matrix of the FBM class.
x	A matrix with the compositional predictors. Zero values are allowed. It may also be a big matrix of the FBM class.
xnew	If you have new data use it, otherwise leave it NULL.
nbcores	The number of cores to use in the case of an FBM class (big) matrix. If you do not know how many cores to use, you may try the command <code>nb_cores()</code> from the <code>bigparallelr</code> package.

### Details

The function performs least squares regression where the beta coefficients are constrained to be positive and sum to 1. We were inspired by the transformation-free linear regression for compositional responses and predictors of Fiksel, Zeger and Datta (2022). Our implementation now uses quadratic programming instead of the function `optim`, and the solution is more accurate and extremely fast.

Big matrices, of FBM class, are now accepted.

### Value

A list including:

mse	The mean squared error.
be	The beta coefficients.
est	The fitted of xnew if xnew is not NULL.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

## References

- Tsagris, M. (2024). Constrained least squares simplicial-simplicial regression. <https://arxiv.org/pdf/2403.19835.pdf>
- Fiksel J., Zeger S. and Datta A. (2022). A transformation-free linear regression for compositional outcomes and predictors. *Biometrics*, 78(3): 974–987.

## See Also

[cv.scls](#), [tflr](#), [scls.indeptest](#), [scrq](#)

## Examples

```
library(MASS)
set.seed(1234)
y <- rdir(214, runif(4, 1, 3))
x <- as.matrix(fgl[, 2:9])
x <- x / rowSums(x)
mod <- scls(y, x)
mod
```

---

The SCLS model with multiple compositional predictors

*The SCLS model with multiple compositional predictors*

---

## Description

The SCLS model with multiple compositional predictors.

## Usage

```
scls2(y, x, wei = FALSE, xnew = NULL)
```

## Arguments

<code>y</code>	A matrix with the compositional data (dependent variable). Zero values are allowed.
<code>x</code>	A list of matrices with the compositional predictors. Zero values are allowed.
<code>wei</code>	Do you want weights among the different simplicial predictors? The default is FALSE.
<code>xnew</code>	If you have new data use it, otherwise leave it NULL.

## Details

The function performs least squares regression where the beta coefficients are constrained to be positive and sum to 1. We were inspired by the transformation-free linear regression for compositional responses and predictors of Fiksel, Zeger and Datta (2020). Our implementation now uses quadratic programming instead of the function `optim`, and the solution is more accurate and extremely fast. This function allows for more than one simplicial predictors and offers the possibility of assigning weights to each simplicial predictor.

**Value**

A list including:

<code>ini.mse</code>	The mean squared error when all simplicial predictors carry equal weight.
<code>ini.be</code>	The beta coefficients when all simplicial predictors carry equal weight.
<code>mse</code>	The mean squared error when the simplicial predictors carry unequal weights.
<code>weights</code>	The weights in a vector form. A vector of length equal to the number of rows of the matrix of coefficients.
<code>am</code>	The vector of weights, one for each simplicia predictor. The length of the vector is equal to the number of simplicial predictors.
<code>est</code>	The fitted of <code>xnew</code> if <code>xnew</code> is not NULL.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Tsagris. M. (2024). Constrained least squares simplicial-simplicial regression. <https://arxiv.org/pdf/2403.19835.pdf>

**See Also**

[cv.scls](#), [tflr](#), [scls.indeptest](#)

**Examples**

```
library(MASS)
set.seed(1234)
y <- rdiri(214, runif(4, 1, 3))
x1 <- as.matrix(fgl[, 2:9])
x <- list()
x[[ 1 ]] <- x1 / rowSums(x1)
x[[ 2 ]] <- Compositional::rdiri(214, runif(4))
mod <- scls2(y, x)
mod
```

---

The TFLR model with multiple compositional predictors

*The TFLR model with multiple compositional predictors*

---

**Description**

The TFLR model with multiple compositional predictors

**Usage**

```
tflr2(y, x, wei = FALSE, xnew = NULL)
```

**Arguments**

<code>y</code>	A matrix with the compositional data (dependent variable). Zero values are allowed.
<code>x</code>	A list of matrices with the compositional predictors. Zero values are allowed.
<code>wei</code>	Do you want weights among the different simplicial predictors? The default is FALSE.
<code>xnew</code>	If you have new data use it, otherwise leave it NULL.

**Details**

The transformation-free linear regression for compositional responses and predictors is implemented. The function to be minimized is  $-\sum_{i=1}^n y_i \log y_i / (X_i B)$ . This is a self implementation of the function that can be found in the package `codalm`. This function allows for more than one simplicial predictors and offers the possibility of assigning weights to each simplicial predictor.

**Value**

A list including:

<code>ini.mse</code>	The mean squared error when all simplicial predictors carry equal weight.
<code>ini.be</code>	The beta coefficients when all simplicial predictors carry equal weight.
<code>mse</code>	The mean squared error when the simplicial predictors carry unequal weights.
<code>weights</code>	The weights in a vector form. A vector of length equal to the number of rows of the matrix of coefficients.
<code>am</code>	The vector of weights, one for each simplicia predictor. The length of the vector is equal to the number of simplicial predictors.
<code>est</code>	The fitted of <code>xnew</code> if <code>xnew</code> is not NULL.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

**References**

Fiksel J., Zeger S. and Datta A. (2022). A transformation-free linear regression for compositional outcomes and predictors. *Biometrics*, 78(3): 974–987.

Tsagris. M. (2024). Constrained least squares simplicial-simplicial regression. <https://arxiv.org/pdf/2403.19835.pdf>

**See Also**

[cv.scls](#), [tflr](#), [scls.indeptest](#)

**Examples**

```

library(MASS)
set.seed(1234)
y <- rdir(214, runif(4, 1, 3))
x1 <- as.matrix(fgl[, 2:9])
x <- list()
x[[ 1 ]] <- x1 / rowSums(x1)
x[[ 2 ]] <- Compositional::rdir(214, runif(4))
mod <- tflr2(y, x)
mod

```

---

The transformation-free linear regression (TFLR) for compositional responses and predictors

*Transformation-free linear regression (TFLR) for compositional responses and predictors*

---

**Description**

Transformation-free linear regression (TFLR) for compositional responses and predictors.

**Usage**

```
tflr(y, x, xnew = NULL)
```

**Arguments**

y	A matrix with the compositional response. Zero values are allowed.
x	A matrix with the compositional predictors. Zero values are in general allowed, but there can be cases when these are problematic.
xnew	If you have new data use it, otherwise leave it NULL.

**Details**

The transformation-free linear regression for compositional responses and predictors is implemented. The function to be minimized is  $-\sum_{i=1}^n y_i \log y_i / (X_i B)$ . This is an efficient self implementation.

**Value**

A list including:

kl	The Kullback-Leibler divergence between the observed and the fitted response compositional data.
be	The beta coefficients.
est	The fitted values of xnew if xnew is not NULL.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

**References**

Fiksel J., Zeger S. and Datta A. (2022). A transformation-free linear regression for compositional outcomes and predictors. *Biometrics*, 78(3): 974–987.

Tsagris. M. (2024). Constrained least squares simplicial-simplicial regression. <https://arxiv.org/pdf/2403.19835.pdf>

**See Also**

[cv.tflr](#), [scls.kl.alfapcr](#)

**Examples**

```
library(MASS)
y <- rdirichlet(214, runif(3, 1, 3))
x <- as.matrix(fgl[, 2:9])
x <- x / rowSums(x)
mod <- tflr(y, x, x)
mod
```

---

Total variability      *Total variability*

---

**Description**

Total variability.

**Usage**

```
totvar(x, a = 0)
```

**Arguments**

x	A numerical matrix with the compositional data.
a	The value of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ the centred log-ratio transformation is used.

**Details**

The  $\alpha$ -transformation is applied and the sum of the variances of the transformed variables is calculated. This is the total variability. Aitchison (1986) used the centred log-ratio transformation, but we have extended it to cover more geometries, via the  $\alpha$ -transformation.

**Value**

The total variability of the data in a given geometry as dictated by the value of  $\alpha$ .

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

**See Also**

[alfa](#), [\link{alfainv}](#), [alfa.profile](#), [alfa.tune](#)

**Examples**

```
x <- as.matrix(iris[, 1:4])
x <- x / rowSums(x)
totvar(x)
```

---

Tuning of the  $\alpha$ -generalised correlations between two compositional datasets

*Tuning of the  $\alpha$ -generalised correlations between two compositional datasets*

---

**Description**

Tuning of the  $\alpha$ -generalised correlations between two compositional datasets.

**Usage**

```
acor.tune(y, x, a, type = "dcor")
```

**Arguments**

<code>y</code>	A matrix with the compositional data.
<code>x</code>	A matrix with the compositional data.
<code>a</code>	The range of values of the power transformation to search for the optimal one. If zero values are present it has to be greater than 0.
<code>type</code>	the type of correlation to compute, the distance correlation ("edist"), the canonical correlation type 1 ("cancor1") or the canonical correlation type 2 ("cancor2"). See details for more information.



**Details**

The  $\alpha$ -transformation is applied to each composition and then, if type="dcor" the distance correlation or the canonical correlation is computed. If type = "cancor1" the function returns the value of  $\alpha$  that maximizes the product of the eigenvalues. If type = "cancor2" the function returns the value of  $\alpha$  that maximizes the the largest eigenvalue.

**Value**

A list including:

alfa	The optimal value of $\alpha$ .
acor	The maximum value of the acor.
runtime	The runtime of the optimization

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain. <https://arxiv.org/pdf/1106.1451.pdf>

**See Also**

[acor](#), [alfa.profile](#), [alfa](#), [alfainv](#)

**Examples**

```
y <- rdiri(30, runif(3) )
x <- rdiri(30, runif(4) )
acor(y, x, a = 0.4)
```

---

Tuning of the bandwidth  $h$  of the kernel using the maximum likelihood cross validation

*Tuning of the bandwidth  $h$  of the kernel using the maximum likelihood cross validation*

---

**Description**

Tuning of the bandwidth  $h$  of the kernel using the maximum likelihood cross validation.

**Usage**

```
mkde.tune( x, low = 0.1, up = 3, s = cov(x) )
```

**Arguments**

<code>x</code>	A matrix with Euclidean (continuous) data.
<code>low</code>	The minimum value to search for the optimal bandwidth value.
<code>up</code>	The maximum value to search for the optimal bandwidth value.
<code>s</code>	A covariance matrix. By default it is equal to the covariance matrix of the data, but can change to a robust covariance matrix, MCD for example.

**Details**

Maximum likelihood cross validation is applied in order to choose the optimal value of the bandwidth parameter. No plot is produced.

**Value**

A list including:

<code>hopt</code>	The optimal bandwidth value.
<code>maximum</code>	The value of the pseudo-log-likelihood at that given bandwidth value.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Giorgos Athineou <gioathineou@gmail.com>.

**References**

Arsalane Chouaib Guidoum (2015). Kernel Estimator and Bandwidth Selection for Density and its Derivatives. The `kedd` R package. <http://cran.r-project.org/web/packages/kedd/vignettes/kedd.pdf>

M.P. Wand and M.C. Jones (1995). Kernel smoothing, pages 91-92.

**See Also**

[mkde](#), [comp.kerncontour](#)

**Examples**

```
library(MASS)
mkde.tune(as.matrix(iris[, 1:4]), c(0.1, 3) )
```

---

Tuning of the divergence based regression for compositional data with compositional data in the covariates side using the alpha-transformation

*Tuning of the divergence based regression for compositional data with compositional data in the covariates side using the  $\alpha$ -transformation*

---

## Description

Tuning of the divergence based regression for compositional data with compositional data in the covariates side using the  $\alpha$ -transformation.

## Usage

```
klalfapcr.tune(y, x, covar = NULL, nfolds = 10, maxk = 50, a = seq(-1, 1, by = 0.1),  
folds = NULL, graph = FALSE, tol = 1e-07, maxiters = 50, seed = NULL)
```

## Arguments

y	A numerical matrix with compositional data with or without zeros.
x	A matrix with the predictor variables, the compositional data. Zero values are allowed.
covar	If you have other continuous covariates put themn here.
nfolds	The number of folds for the K-fold cross validation, set to 10 by default.
maxk	The maximum number of principal components to check.
a	The value of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ the isometric log-ratio transformation is applied.
folds	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.
graph	If graph is TRUE (default value) a plot will appear.
tol	The tolerance value to terminate the Newton-Raphson procedure.
maxiters	The maximum number of Newton-Raphson iterations.
seed	You can specify your own seed number here or leave it NULL.

## Details

The M-fold cross validation is performed in order to select the optimal values for  $\alpha$  and k, the number of principal components. The  $\alpha$ -transformation is applied to the compositional data first, the first k principal component scores are calculated and used as predictor variables for the Kullback-Leibler divergence based regression model. This procedure is performed M times during the M-fold cross validation.

**Value**

A list including:

mspe	A list with the KL divergence for each value of $\alpha$ and $k$ in every fold.
performance	A matrix with the KL divergence for each value of $\alpha$ averaged over all folds. If graph is set to TRUE this matrix is plotted.
best.perf	The minimum KL divergence.
params	The values of $\alpha$ and $k$ corresponding to the minimum KL divergence.

**Author(s)**

Initial code by Abdulaziz Alenazi. Modifications by Michail Tsagris.

R implementation and documentation: Abdulaziz Alenazi <a.alenazi@nbu.edu.sa> and Michail Tsagris <mtsagris@uoc.gr>.

**References**

- Alenazi A. (2019). Regression for compositional data with compositional data as predictor variables with or without zero values. *Journal of Data Science*, 17(1): 219–238. <https://jds-online.org/journal/JDS/article/136/file/pdf>
- Tsagris M. (2015). Regression analysis with compositional data containing zero values. *Chilean Journal of Statistics*, 6(2): 47–57. <http://arxiv.org/pdf/1508.01913v1.pdf>
- Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In *Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain*. <http://arxiv.org/pdf/1106.1451.pdf>

**See Also**

[kl.alfapcr](#), [cv.tflr](#), [glm.pcr](#), [alfapcr.tune](#)

**Examples**

```
library(MASS)
y <- rdir( 214, runif(4, 1, 3) )
x <- as.matrix( fgl[, 2:9] )
x <- x / rowSums(x)
mod <- klalfapcr.tune(y = y, x = x, a = c(0.7, 0.8) )
mod
```

---

Tuning of the  $k$ -NN algorithm for compositional data

*Tuning of the  $k$ -NN algorithm for compositional data*

---

**Description**

Tuning of the  $k$ -NN algorithm for compositional data with and without using the power or the  $\alpha$ -transformation. In addition, estimation of the rate of correct classification via  $K$ -fold cross-validation.

**Usage**

```
compknn.tune(x, ina, nfolds = 10, k = 2:5, mesos = TRUE,
a = seq(-1, 1, by = 0.1), apostasi = "ESOV", folds = NULL,
stratified = TRUE, seed = NULL, graph = FALSE)
```

```
alfaknn.tune(x, ina, nfolds = 10, k = 2:5, mesos = TRUE,
a = seq(-1, 1, by = 0.1), apostasi = "euclidean", rann = FALSE,
folds = NULL, stratified = TRUE, seed = NULL, graph = FALSE)
```

```
aitknn.tune(x, ina, nfolds = 10, k = 2:5, mesos = TRUE,
a = seq(-1, 1, by = 0.1), apostasi = "euclidean", rann = FALSE,
folds = NULL, stratified = TRUE, seed = NULL, graph = FALSE)
```

**Arguments**

x	A matrix with the available compositional data. Zeros are allowed, but you must be careful to choose strictly positive values of $\alpha$ or not to set <code>apostasi= "Ait"</code> .
ina	A group indicator variable for the available data.
nfolds	The number of folds to be used. This is taken into consideration only if the folds argument is not supplied.
k	A vector with the nearest neighbours to consider.
mesos	This is used in the non standard algorithm. If TRUE, the arithmetic mean of the distances is calculated, otherwise the harmonic mean is used (see details).
a	A grid of values of $\alpha$ to be used only if the distance chosen allows for it.
apostasi	The type of distance to use. For the <code>compk.knn</code> this can be one of the following: "ESOV", "taxicab", "Ait", "Hellinger", "angular" or "CS". See the references for them. For the <code>alfa.knn</code> this can be either "euclidean" or "manhattan".
rann	If you have large scale datasets and want a faster k-NN search, you can use kd-trees implemented in the R package "Rnanoflann". In this case you must set this argument equal to TRUE. Note however, that in this case, the only available distance is by default "euclidean".
folds	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.
stratified	Do you want the folds to be created in a stratified way? TRUE or FALSE.
seed	You can specify your own seed number here or leave it NULL.
graph	If set to TRUE a graph with the results will appear.

**Details**

The k-NN algorithm is applied for the compositional data. There are many metrics and possibilities to choose from. The algorithm finds the k nearest observations to a new observation and allocates it to the class which appears most times in the neighbours.

**Value**

A list including:

per	A matrix or a vector (depending on the distance chosen) with the averaged over all folds rates of correct classification for all hyper-parameters ( $\alpha$ and $k$ ).
performance	The estimated rate of correct classification.
best_a	The best value of $\alpha$ . This is returned for "ESOV" and "taxicab" only.
best_k	The best number of nearest neighbours.
runtime	The run time of the cross-validation procedure.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Giorgos Athineou <gioathineou@gmail.com>.

**References**

- Tsagris, Michail (2014). The *k*-NN algorithm for compositional data: a revised approach with and without zero values present. *Journal of Data Science*, 12(3): 519–534. <https://arxiv.org/pdf/1506.05216.pdf>
- Friedman Jerome, Trevor Hastie and Robert Tibshirani (2009). *The elements of statistical learning*, 2nd edition. Springer, Berlin
- Tsagris M., Preston S. and Wood A.T.A. (2016). Improved classification for compositional data using the  $\alpha$ -transformation. *Journal of Classification*, 33(2): 243–261. <http://arxiv.org/pdf/1106.1451.pdf>
- Connie Stewart (2017). An approach to measure distance between compositional diet estimates containing essential zeros. *Journal of Applied Statistics* 44(7): 1137–1152.
- Clarotto L., Allard D. and Menafoglio A. (2022). A new class of  $\alpha$ -transformations for the spatial analysis of Compositional Data. *Spatial Statistics*, 47.
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**See Also**

[comp.knn](#), [alfarda.tune](#), [cv.dda](#), [cv.compnb](#)

**Examples**

```
x <- as.matrix(iris[, 1:4])
x <- x/ rowSums(x)
ina <- iris[, 5]
mod1 <- compknn.tune(x, ina, a = seq(1, 1, by = 0.1) )
mod2 <- alfaknn.tune(x, ina, a = seq(-1, 1, by = 0.1) )
```

---

Tuning of the projection pursuit regression for compositional data  
*Tuning of the projection pursuit regression for compositional data*

---

**Description**

Tuning of the projection pursuit regression for compositional data.

**Usage**

```
compppr.tune(y, x, nfolds = 10, folds = NULL, seed = NULL,  
nterms = 1:10, type = "alr", yb = NULL )
```

**Arguments**

y	A matrix with the available compositional data, but zeros are not allowed.
x	A matrix with the continuous predictor variables.
nfolds	The number of folds to use.
folds	If you have the list with the folds supply it here.
seed	You can specify your own seed number here or leave it NULL.
nterms	The number of terms to try in the projection pursuit regression.
type	Either "alr" or "ilr" corresponding to the additive or the isometric log-ratio transformation respectively.
yb	If you have already transformed the data using a log-ratio transformation put it here. Otherwise leave it NULL.

**Details**

The function performs tuning of the projection pursuit regression algorithm.

**Value**

A list including:

kl	The average Kullback-Leibler divergence.
perf	The average Kullback-Leibler divergence.
runtime	The run time of the cross-validation procedure.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

## References

Friedman, J. H. and Stuetzle, W. (1981). Projection pursuit regression. *Journal of the American Statistical Association*, 76, 817-823. doi: 10.2307/2287576.

## See Also

[comp.ppr](#), [aknnreg.tune](#), [akernreg.tune](#)

## Examples

```
y <- as.matrix(iris[, 1:3])
y <- y/ rowSums(y)
x <- iris[, 4]
mod <- compppr.tune(y, x)
```

---

Tuning of the projection pursuit regression with compositional predictor variables

*Tuning of the projection pursuit regression with compositional predictor variables*

---

## Description

Tuning of the projection pursuit regression with compositional predictor variables.

## Usage

```
pprcomp.tune(y, x, nfolds = 10, folds = NULL, seed = NULL,
nterms = 1:10, type = "log", graph = FALSE)
```

## Arguments

y	A numerical vector with the continuous variable.
x	A matrix with the available compositional data, but zeros are not allowed.
nfolds	The number of folds to use.
folds	If you have the list with the folds supply it here.
seed	You can specify your own seed number here or leave it NULL.
nterms	The number of terms to try in the projection pursuit regression.
type	Either "alr" or "log" corresponding to the additive log-ratio transformation or the logarithm applied to the compositional predictor variables.
graph	If graph is TRUE (default value) a filled contour plot will appear.

## Details

The function performs tuning of the projection pursuit regression algorithm with compositional predictor variables.



## Value

A list including:

<code>runtime</code>	The run time of the cross-validation procedure.
<code>mse</code>	The mean squared error of prediction for each number of terms.
<code>opt.nterms</code>	The number of terms corresponding to the minimum mean squared error of prediction.
<code>opt.alpha</code>	The value of $\alpha$ corresponding to the minimum mean squared error of prediction.
<code>performance</code>	The minimum mean squared error of prediction.

## Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

## References

Friedman, J. H. and Stuetzle, W. (1981). Projection pursuit regression. *Journal of the American Statistical Association*, 76, 817-823. doi: 10.2307/2287576.

## See Also

[pprcomp](#), [ice.pprcomp](#), [alfapcr.tune](#), [compppr.tune](#)

## Examples

```
x <- as.matrix(iris[, 2:4])
x <- x/ rowSums(x)
y <- iris[, 1]
mod <- pprcomp.tune(y, x)
```

---

Tuning of the projection pursuit regression with compositional  
predictor variables using the alpha-transformation

*Tuning of the projection pursuit regression with compositional predictor  
variables using the  $\alpha$ -transformation*

---

## Description

Tuning of the projection pursuit regression with compositional predictor variables using the  $\alpha$ -transformation.

## Usage

```
alfapprcomp.tune(y, x, nfolds = 10, folds = NULL, seed = NULL,  
nterms = 1:10, a = seq(-1, 1, by = 0.1), graph = FALSE)
```

### Arguments

y	A numerical vector with the continuous variable.
x	A matrix with the available compositional data. Zeros are allowed.
nfolds	The number of folds to use.
folds	If you have the list with the folds supply it here.
seed	You can specify your own seed number here or leave it NULL.
nterms	The number of terms to try in the projection pursuit regression.
a	A vector with the values of $\alpha$ for the $\alpha$ -transformation.
graph	If graph is TRUE (default value) a filled contour plot will appear.

### Details

The function performs tuning of the projection pursuit regression algorithm with compositional predictor variables using the  $\alpha$ -transformation.

### Value

A list including:

runtime	The run time of the cross-validation procedure.
mse	The mean squared error of prediction for each number of terms.
opt.terms	The number of terms corresponding to the minimum mean squared error of prediction.
opt.alpha	The value of $\alpha$ corresponding to the minimum mean squared error of prediction.
performance	The minimum mean squared error of prediction.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

### References

Friedman, J. H. and Stuetzle, W. (1981). Projection pursuit regression. *Journal of the American Statistical Association*, 76, 817-823. doi: 10.2307/2287576.

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In *Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain*. <https://arxiv.org/pdf/1106.1451.pdf>

### See Also

[alfa.pprcomp](#), [pprcomp.tune](#), [compppr.tune](#)

### Examples

```
x <- as.matrix(iris[, 2:4])
x <- x / rowSums(x)
y <- iris[, 1]
mod <- alfapcrcomp.tune( y, x, a = c(0, 0.5, 1) )
```

---

Tuning the number of PCs in the PCR with compositional data using the alpha-transformation

*Tuning the number of PCs in the PCR with compositional data using the  $\alpha$ -transformation*

---

### Description

This is a cross-validation procedure to decide on the number of principal components when using regression with compositional data (as predictor variables) using the  $\alpha$ -transformation.

### Usage

```
alfapcr.tune(y, x, model = "gaussian", nfold = 10, maxk = 50, a = seq(-1, 1, by = 0.1),
  folds = NULL, ncores = 1, graph = TRUE, col.nu = 15, seed = NULL)
```

### Arguments

y	A vector with either continuous, binary or count data.
x	A matrix with the predictor variables, the compositional data. Zero values are allowed.
model	The type of regression model to fit. The possible values are "gaussian", "binomial" and "poisson".
nfold	The number of folds for the K-fold cross validation, set to 10 by default.
maxk	The maximum number of principal components to check.
a	A vector with a grid of values of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ the isometric log-ratio transformation is applied.
folds	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.
ncores	How many cores to use. If you have heavy computations or do not want to wait for long time more than 1 core (if available) is suggested. It is advisable to use it if you have many observations and or many variables, otherwise it will slow down the process.
graph	If graph is TRUE (default value) a filled contour plot will appear.
col.nu	A number parameter for the filled contour plot, taken into account only if graph is TRUE.
seed	You can specify your own seed number here or leave it NULL.

**Details**

The  $\alpha$ -transformation is applied to the compositional data first and the function "pcr.tune" or "glm-pcr.tune" is called.

**Value**

If graph is TRUE a filled contour will appear. A list including:

mspe	The MSPE where rows correspond to the $\alpha$ values and the columns to the number of principal components.
best.par	The best pair of $\alpha$ and number of principal components.
performance	The minimum mean squared error of prediction.
runtime	The time required by the cross-validation procedure.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Tsagris M. (2015). Regression analysis with compositional data containing zero values. Chilean Journal of Statistics, 6(2): 47-57. <https://arxiv.org/pdf/1508.01913v1.pdf>

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain. <https://arxiv.org/pdf/1106.1451.pdf>

Jolliffe I.T. (2002). Principal Component Analysis.

**See Also**

[alfa](#), [profile](#), [alfa.pcr](#), [pcr.tune](#), [glmPCR.tune](#), [glm](#)

**Examples**

```
library(MASS)
y <- as.vector(fg1[, 1])
x <- as.matrix(fg1[, 2:9])
x <- x/ rowSums(x)
mod <- alfapcr.tune(y, x, nolds = 10, maxk = 50, a = seq(-1, 1, by = 0.1) )
```

---

Tuning the parameters of the regularised discriminant analysis

*Tuning the parameters of the regularised discriminant analysis*

---

## Description

Tuning the parameters of the regularised discriminant analysis for Euclidean data.

## Usage

```
rda.tune(x, ina, nfolds = 10, gam = seq(0, 1, by = 0.1), del = seq(0, 1, by = 0.1),
ncores = 1, folds = NULL, stratified = TRUE, seed = NULL)
```

## Arguments

x	A matrix with the data.
ina	A group indicator variable for the available data.
nfolds	The number of folds in the cross validation.
gam	A grid of values for the $\gamma$ parameter as defined in Tsagris et al. (2016).
del	A grid of values for the $\delta$ parameter as defined in Tsagris et al. (2016).
ncores	The number of cores to use. If more than 1, parallel computing will take place. It is advisable to use it if you have many observations and/or many variables, otherwise it will slow down the process.
folds	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.
stratified	Do you want the folds to be created in a stratified way? TRUE or FALSE.
seed	You can specify your own seed number here or leave it NULL.

## Details

Cross validation is performed to select the optimal parameters for the regularised discriminant analysis and also estimate the rate of accuracy.

The covariance matrix of each group is calculated and then the pooled covariance matrix. The spherical covariance matrix consists of the average of the pooled variances in its diagonal and zeros in the off-diagonal elements.  $\text{gam}$  is the weight of the pooled covariance matrix and  $1-\text{gam}$  is the weight of the spherical covariance matrix,  $S_a = \text{gam} * S_p + (1-\text{gam}) * s_p$ . Then it is a compromise between LDA and QDA.  $\text{del}$  is the weight of  $S_a$  and  $1-\text{del}$  the weight of each group covariance matrix.

## Value

A list including: If  $\text{graph}$  is TRUE a plot of a heatmap of the performance  $s$  will appear.

per	An array with the estimate rate of correct classification for every fold. For each of the $M$ matrices, the row values correspond to $\text{gam}$ and the columns to the $\text{del}$ parameter.
-----	--

percent	A matrix with the mean estimated rates of correct classification. The row values correspond to gam and the columns to the del parameter.
se	A matrix with the standard error of the mean estimated rates of correct classification. The row values correspond to gam and the columns to the del parameter.
result	The estimated rate of correct classification along with the best gam and del parameters.
runtime	The time required by the cross-validation procedure.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Friedman J.H. (1989): Regularized Discriminant Analysis. *Journal of the American Statistical Association* 84(405): 165–175.

Friedman Jerome, Trevor Hastie and Robert Tibshirani (2009). *The elements of statistical learning*, 2nd edition. Springer, Berlin.

Tsagris M., Preston S. and Wood A.T.A. (2016). Improved classification for compositional data using the  $\alpha$ -transformation. *Journal of Classification*, 33(2): 243–261.

**See Also**

[rda](#)

**Examples**

```
mod <- rda.tune(as.matrix(iris[, 1:4]), iris[, 5], gam = seq(0, 1, by = 0.2),
del = seq(0, 1, by = 0.2) )
mod
```

---

Tuning the principal components with GLMs

*Tuning the principal components with GLMs*

---

**Description**

Tuning the number of principal components in the generalised linear models.

**Usage**

```
pcr.tune(y, x, nfolds = 10, maxk = 50, folds = NULL, ncores = 1,
seed = NULL, graph = TRUE)
```

```
glmpr.tune(y, x, nfolds = 10, maxk = 10, folds = NULL, ncores = 1,
seed = NULL, graph = TRUE)
```

```
multinompcr.tune(y, x, nfolds = 10, maxk = 10, folds = NULL, ncores = 1,
seed = NULL, graph = TRUE)
```

**Arguments**

y	A real valued vector for "pcr.tune". A real valued vector for the "glmpr.tune" with either two numbers, 0 and 1 for example, for the binomial regression or with positive discrete numbers for the poisson. For the "multinompcr.tune" a vector or a factor with more than just two values. This is a multinomial regression.
x	A matrix with the predictor variables, they have to be continuous.
nfolds	The number of folds in the cross validation.
maxk	The maximum number of principal components to check.
folds	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.
ncores	The number of cores to use. If more than 1, parallel computing will take place. It is advisable to use it if you have many observations and or many variables, otherwise it will slow down th process.
seed	You can specify your own seed number here or leave it NULL.
graph	If graph is TRUE a plot of the performance for each fold along the values of $\alpha$ will appear.

**Details**

Cross validation is performed to select the optimal number of principal components in the GLMs or the multinomial regression. This is used by [alfapcr.tune](#).

**Value**

If graph is TRUE a plot of the performance versus the number of principal components will appear. A list including:

mSP	A matrix with the mean deviance of prediction or mean accuracy for every fold.
mpd	A vector with the mean deviance of prediction or mean accuracy, each value corresponds to a number of principal components.
k	The number of principal components which minimizes the deviance or maximises the accuracy.
performance	The optimal performance, MSE for the linea regression, minimum deviance for the GLMs and maximum accuracy for the multinomial regression.
runtime	The time required by the cross-validation procedure.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Aguilera A.M., Escabias M. and Valderrama M.J. (2006). Using principal components for estimating logistic regression with high-dimensional multicollinear data. *Computational Statistics & Data Analysis* 50(8): 1905-1924.

Jolliffe I.T. (2002). *Principal Component Analysis*.

**See Also**

[pcr.tune](#), [glm.pcr](#), [alfa.pcr](#), [alfapcr.tune](#)

**Examples**

```
library(MASS)
x <- as.matrix(fg1[, 2:9])
y <- rpois(214, 10)
glmPCR.tune(y, x, nfolds = 10, maxk = 20, folds = NULL, ncores = 1)
```

---

Tuning the value of alpha in the alpha-regression

*Tuning the value of  $\alpha$  in the  $\alpha$ -regression*

---

**Description**

Tuning the value of  $\alpha$  in the  $\alpha$ -regression.

**Usage**

```
alfareg.tune(y, x, a = seq(0.1, 1, by = 0.1), nfolds = 10,
folds = NULL, nc = 1, seed = NULL, graph = FALSE)
```

**Arguments**

y	A matrix with compositional data. zero values are allowed.
x	A matrix with the continuous predictor variables or a data frame including categorical predictor variables.
a	The value of the power transformation, it has to be between -1 and 1. If zero values are present it has to be greater than 0. If $\alpha = 0$ the isometric log-ratio transformation is applied.
nfolds	The number of folds to split the data.
folds	If you have the list with the folds supply it here. You can also leave it NULL and it will create folds.



nc	The number of cores to use. IF you have a multicore computer it is advisable to use more than 1. It makes the procedure faster. It is advisable to use it if you have many observations and or many variables, otherwise it will slow down th process.
seed	You can specify your own seed number here or leave it NULL.
graph	If graph is TRUE a plot of the performance for each fold along the values of $\alpha$ will appear.

### Details

The  $\alpha$ -transformation is applied to the compositional data and the numerical optimisation is performed for the regression, unless  $\alpha = 0$ , where the coefficients are available in closed form.

### Value

A plot of the estimated Kullback-Leibler divergences (multiplied by 2) along the values of  $\alpha$  (if graph is set to TRUE). A list including:

runtime	The runtime required by the cross-validation.
kula	A matrix with twice the Kullback-Leibler divergence of the observed from the fitted values. Each row corresponds to a fold and each column to a value of $\alpha$ . The average over the columns equal the next argument, "kl".
kl	A vector with twice the Kullback-Leibler divergence of the observed from the fitted values. Every value corresponds to a value of $\alpha$ .
opt	The optimal value of $\alpha$ .
value	The minimum value of twice the Kullback-Leibler.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr> and Giorgos Athineou <gioathineou@gmail.com>.

### References

Tsagris M. (2015). Regression analysis with compositional data containing zero values. Chilean Journal of Statistics, 6(2): 47-57. <https://arxiv.org/pdf/1508.01913v1.pdf>

Tsagris M.T., Preston S. and Wood A.T.A. (2011). A data-based power transformation for compositional data. In Proceedings of the 4th Compositional Data Analysis Workshop, Girona, Spain. <https://arxiv.org/pdf/1106.1451.pdf>

### See Also

[alfa.reg](#), [alfa](#)

**Examples**

```
library(MASS)
y <- as.matrix(fg1[1:40, 2:4])
y <- y / rowSums(y)
x <- as.vector(fg1[1:40, 1])
mod <- alfareg.tune(y, x, a = seq(0, 1, by = 0.1), nfolds = 5)
```

---

Two-sample test of high-dimensional means for compositional data

*Two-sample test of high-dimensional means for compositional data*

---

**Description**

Two-sample test of high-dimensional means for compositional data.

**Usage**

```
hd.meantest2(y1, y2, R = 1)
```

**Arguments**

y1	A matrix containing the compositional data of the first group.
y2	A matrix containing the compositional data of the second group.
R	If R is 1 no bootstrap calibration is performed and the asymptotic p-value is returned. If R is greater than 1, the bootstrap p-value is returned.

**Details**

A two sample for high dimensional mean vectors of compositional data is implemented. See references for more details.

**Value**

A vector with the test statistic value and its associated (bootstrap) p-value.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Cao Y., Lin W. and Li H. (2018). Two-sample tests of high-dimensional means for compositional data. *Biometrika*, 105(1): 115-132.

**See Also**

[comp.test](#)

**Examples**

```
m <- runif(200, 10, 15)
x1 <- rdir(100, m)
x2 <- rdir(100, m)
hd.meantest2(x1, x2)
```

---

Unconstrained GLMs with compositional predictor variables

*Unconstrained GLMs with compositional predictor variables*

---

**Description**

Unconstrained GLMs with compositional predictor variables.

**Usage**

```
ulc.glm(y, x, z = NULL, model = "logistic", xnew = NULL, znew = NULL)
```

**Arguments**

y	A numerical vector containing the response variable values. This is either a binary variable or a vector with counts.
x	A matrix with the predictor variables, the compositional data. No zero values are allowed.
z	A matrix, data.frame, factor or a vector with some other covariate(s).
model	For the <code>ulc.glm()</code> , this can be either "logistic" or "poisson".
xnew	A matrix containing the new compositional data whose response is to be predicted. If you have no new data, leave this NULL as is by default.
znew	A matrix, data.frame, factor or a vector with the values of some other covariate(s). If you have no new data, leave this NULL as is by default.

**Details**

The function performs the unconstrained log-contrast logistic or Poisson regression model. The logarithm of the compositional predictor variables is used (hence no zero values are allowed). The response variable is linked to the log-transformed data **without** the constraint that the sum of the regression coefficients equals 0. If you want the regression without the sum-to-zero constraints see [lc.glm](#). Extra predictor variables are allowed as well, for instance categorical or continuous.

**Value**

A list including:

devi	The residual deviance of the logistic or Poisson regression model.
be	The unconstrained regression coefficients. Their sum does not equal 0.
est	If the arguments "xnew" and znew were given these are the predicted or estimated values, otherwise it is NULL.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

Lu J., Shi P., and Li H. (2019). Generalized linear models with linear constraints for microbiome compositional data. *Biometrics*, 75(1): 235–244.

**See Also**

[lc.glm](#), [lc.glm2](#), [ulc.glm2](#), [lcglm.aov](#)

**Examples**

```
y <- rbinom(150, 1, 0.5)
x <- rdiri(150, runif(3, 1,3))
mod <- ulc.glm(y, x)
```

---

Unconstrained linear regression with compositional predictor variables

*Unconstrained linear regression with compositional predictor variables*

---

**Description**

Unconstrained linear regression with compositional predictor variables.

**Usage**

```
ulc.reg(y, x, z = NULL, xnew = NULL, znew = NULL)
```

**Arguments**

y	A numerical vector containing the response variable values. This must be a continuous variable.
x	A matrix with the predictor variables, the compositional data. No zero values are allowed.
z	A matrix, data.frame, factor or a vector with some other covariate(s).
xnew	A matrix containing the new compositional data whose response is to be predicted. If you have no new data, leave this NULL as is by default.
znew	A matrix, data.frame, factor or a vector with the values of some other covariate(s). If you have no new data, leave this NULL as is by default.

## Details

The function performs the unconstrained log-contrast regression model as opposed to the log-contrast regression described in Aitchison (2003), pg. 84-85. The logarithm of the compositional predictor variables is used (hence no zero values are allowed). The response variable is linked to the log-transformed data **without** the constraint that the sum of the regression coefficients equals 0. If you want the regression model with the sum-to-zero constraints see [lc.reg](#). Extra predictors variables are allowed as well, for instance categorical or continuous.

## Value

A list including:

<code>be</code>	The unconstrained regression coefficients. Their sum does not equal 0.
<code>covbe</code>	If covariance matrix of the constrained regression coefficients.
<code>va</code>	The estimated regression variance.
<code>residuals</code>	The vector of residuals.
<code>est</code>	If the arguments "xnew" and "znew" were given these are the predicted or estimated values, otherwise it is NULL.

## Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

## References

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

## See Also

[lc.reg](#), [lcreg.aov](#), [lc.reg2](#), [ulc.reg2](#), [alfa.pcr](#), [alfa.knn.reg](#)

## Examples

```
y <- iris[, 1]
x <- as.matrix(iris[, 2:4])
x <- x / rowSums(x)
mod1 <- ulc.reg(y, x)
mod2 <- ulc.reg(y, x, z = iris[, 5])
```

---

Unconstrained linear regression with multiple compositional predictors

*Unconstrained linear regression with multiple compositional predictors*

---

## Description

Unconstrained linear regression with multiple compositional predictors.

## Usage

```
ulc.reg2(y, x, z = NULL, xnew = NULL, znew = NULL)
```

## Arguments

y	A numerical vector containing the response variable values. This must be a continuous variable.
x	A list with multiple matrices with the predictor variables, the compositional data. No zero values are allowed.
z	A matrix, data.frame, factor or a vector with some other covariate(s).
xnew	A matrix containing a list with multiple matrices with compositional data whose response is to be predicted. If you have no new data, leave this NULL as is by default.
znew	A matrix, data.frame, factor or a vector with the values of some other covariate(s). If you have no new data, leave this NULL as is by default.

## Details

The function performs the unconstrained log-contrast regression model as opposed to the log-contrast regression described in Aitchison (2003), pg. 84-85. The logarithm of the compositional predictor variables is used (hence no zero values are allowed). The response variable is linked to the log-transformed data **without** the constraint that the sum of the regression coefficients equals 0. If you want the regression model with the sum-to-zero constraints see [lc.reg2](#). Extra predictor variables are allowed as well, for instance categorical or continuous. Similarly to [lc.reg2](#) there are multiple compositions treated as predictor variables.

## Value

A list including:

be	The unconstrained regression coefficients. Their sum for each composition does not equal 0.
covbe	If covariance matrix of the constrained regression coefficients.
va	The estimated regression variance.
residuals	The vector of residuals.

`est` If the arguments "xnew" and "znew" were given these are the predicted or estimated values, otherwise it is NULL.

### Author(s)

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

### References

Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.

Xiaokang Liu, Xiaomei Cong, Gen Li, Kendra Maas and Kun Chen (2020). Multivariate Log-Contrast Regression with Sub-Compositional Predictors: Testing the Association Between Preterm Infants' Gut Microbiome and Neurobehavioral Outcome.

### See Also

[lc.reg2](#), [ulc.reg](#), [lc.reg](#), [alfa.pcr](#), [alfa.knn.reg](#)

### Examples

```
y <- iris[, 1]
x <- list()
x1 <- as.matrix(iris[, 2:4])
x1 <- x1 / rowSums(x1)
x[[ 1 ]] <- x1
x[[ 2 ]] <- rdir(150, runif(4) )
x[[ 3 ]] <- rdir(150, runif(5) )
mod <- lc.reg2(y, x)
```

---

Unconstrained logistic or Poisson regression with multiple  
compositional predictors

*Unconstrained logistic or Poisson regression with multiple compositional predictors*

---

### Description

Unconstrained logistic or Poisson regression with multiple compositional predictors.

### Usage

```
ulc.glm2(y, x, z = NULL, model = "logistic", xnew = NULL, znew = NULL)
```

**Arguments**

y	A numerical vector containing the response variable values. This is either a binary variable or a vector with counts.
x	A list with multiple matrices with the predictor variables, the compositional data. No zero values are allowed.
z	A matrix, data.frame, factor or a vector with some other covariate(s).
model	This can be either "logistic" or "poisson".
xnew	A matrix containing a list with multiple matrices with compositional data whose response is to be predicted. If you have no new data, leave this NULL as is by default.
znew	A matrix, data.frame, factor or a vector with the values of some other covariate(s). If you have no new data, leave this NULL as is by default.

**Details**

The function performs the unconstrained log-contrast logistic or Poisson regression model. The logarithm of the compositional predictor variables is used (hence no zero values are allowed). The response variable is linked to the log-transformed data **without** the constraint that the sum of the regression coefficients equals 0. If you want the regression without the sum-to-zero constraints see [lc.glm2](#). Extra predictor variables are allowed as well, for instance categorical or continuous.

**Value**

A list including:

devi	The residual deviance of the logistic or Poisson regression model.
be	The unconstrained regression coefficients. Their sum does not equal 0.
est	If the arguments "xnew" and znew were given these are the predicted or estimated values, otherwise it is NULL.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

**References**

- Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.
- Lu J., Shi P., and Li H. (2019). Generalized linear models with linear constraints for microbiome compositional data. *Biometrics*, 75(1): 235–244.

**See Also**

[lc.glm2](#), [ulc.glm](#), [lc.glm](#)



## Examples

```
y <- rbinom(150, 1, 0.5)
x <- list()
x1 <- as.matrix(iris[, 2:4])
x1 <- x1 / rowSums(x1)
x[[ 1 ]] <- x1
x[[ 2 ]] <- rdir(150, runif(4) )
x[[ 3 ]] <- rdir(150, runif(5) )
mod <- ulc.glm2(y, x)
```

---

Unconstrained quantile regression with compositional predictor variables

*Unconstrained quantile regression with compositional predictor variables*

---

## Description

Unconstrained quantile regression with compositional predictor variables.

## Usage

```
ulc.rq(y, x, z = NULL, tau = 0.5, xnew = NULL, znew = NULL)
```

## Arguments

y	A numerical vector containing the response variable values.
x	A matrix with the predictor variables, the compositional data. No zero values are allowed.
z	A matrix, data.frame, factor or a vector with some other covariate(s).
tau	The quantile to be estimated, a number between 0 and 1.
xnew	A matrix containing the new compositional data whose response is to be predicted. If you have no new data, leave this NULL as is by default.
znew	A matrix, data.frame, factor or a vector with the values of some other covariate(s). If you have no new data, leave this NULL as is by default.

## Details

The function performs the unconstrained log-contrast quantile regression model. The logarithm of the compositional predictor variables is used (hence no zero values are allowed). The response variable is linked to the log-transformed data **without** the constraint that the sum of the regression coefficients equals 0. If you want the regression without the sum-to-zero constraints see [lc.rq](#). Extra predictor variables are allowed as well, for instance categorical or continuous.

**Value**

A list including:

<code>mod</code>	The object as returned by the function <code>quantreg::rq()</code> . This is useful for hypothesis testing purposes.
<code>be</code>	The unconstrained regression coefficients. Their sum does not equal 0.
<code>est</code>	If the arguments "xnew" and znew were given these are the predicted or estimated values, otherwise it is NULL.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

- Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.
- Koenker R. W. and Bassett G. W. (1978). Regression Quantiles, *Econometrica*, 46(1): 33–50.
- Koenker R. W. and d'Orey V. (1987). Algorithm AS 229: Computing Regression Quantiles. *Applied Statistics*, 36(3): 383–393.

**See Also**

[lc.glm](#), [lc.glm2](#), [ulc.glm2](#), [lcglm.aov](#)

**Examples**

```
y <- rnorm(150)
x <- rdir(150, runif(3, 1,3))
mod <- ulc.rq(y, x)
```

---

Unconstrained quantile regression with multiple compositional predictors

*Unconstrained quantile regression with multiple compositional predictors*

---

**Description**

Unconstrained quantile regression with multiple compositional predictors.

**Usage**

```
ulc.rq2(y, x, z = NULL, tau = 0.5, xnew = NULL, znew = NULL)
```

**Arguments**

y	A numerical vector containing the response variable values.
x	A list with multiple matrices with the predictor variables, the compositional data. No zero values are allowed.
z	A matrix, data.frame, factor or a vector with some other covariate(s).
tau	The quantile to be estimated, a number between 0 and 1.
xnew	A matrix containing a list with multiple matrices with compositional data whose response is to be predicted. If you have no new data, leave this NULL as is by default.
znew	A matrix, data.frame, factor or a vector with the values of some other covariate(s). If you have no new data, leave this NULL as is by default.

**Details**

The function performs the unconstrained log-contrast quantile regression model. The logarithm of the compositional predictor variables is used (hence no zero values are allowed). The response variable is linked to the log-transformed data **without** the constraint that the sum of the regression coefficients equals 0. If you want the regression without the sum-to-zero constraints see [lc.rq2](#). Extra predictors variables are allowed as well, for instance categorical or continuous.

**Value**

A list including:

mod	The object as returned by the function <code>quantreg::rq()</code> . This is useful for hypothesis testing purposes.
be	The unconstrained regression coefficients. Their sum does not equal 0.
est	If the arguments "xnew" and znew were given these are the predicted or estimated values, otherwise it is NULL.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <[mtsagris@uoc.gr](mailto:mtsagris@uoc.gr)>.

**References**

- Aitchison J. (1986). The statistical analysis of compositional data. Chapman & Hall.
- Koenker R. W. and Bassett G. W. (1978). Regression Quantiles, *Econometrica*, 46(1): 33–50.
- Koenker R. W. and d’Orey V. (1987). Algorithm AS 229: Computing Regression Quantiles. *Applied Statistics*, 36(3): 383–393.

**See Also**

[ulc.rq](#), [lc.rq](#)

**Examples**

```
y <- rnorm(150)
x <- list()
x1 <- as.matrix(iris[, 2:4])
x1 <- x1 / rowSums(x1)
x[[ 1 ]] <- x1
x[[ 2 ]] <- rdir(150, runif(4) )
x[[ 3 ]] <- rdir(150, runif(5) )
mod <- ulc.rq2(y, x)
```

---

Unit-Weibull regression models for proportions

*Unit-Weibull regression models for proportions*

---

**Description**

Unit-Weibull regression models for proportions.

**Usage**

```
unitweib.reg(y, x, tau = 0.5)
```

**Arguments**

y	A numerical vector proportions. 0s and 1s are allowed.
x	A matrix or a data frame with the predictor variables.
tau	The quantile to be used for estimation. The default value is 0.5 yielding the median.

**Details**

See the reference paper.

**Value**

A list including:

loglik	The loglikelihood of the regression model.
info	A matrix with all estimated parameters, their standard error, their Wald-statistic and its associated p-value.

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Mazucheli J., Menezes A. F. B., Fernandes L. B., de Oliveira R. P. and Ghitany M. E. (2020). The unit-Weibull distribution as an alternative to the Kumaraswamy distribution for the modeling of quantiles conditional on covariates. *Journal of Applied Statistics*, 47(6): 954–974.

**See Also**

[propreg](#), [beta.reg](#)

**Examples**

```
y <- exp( - rweibull(100, 1, 1) )
x <- matrix( rnorm(100 * 2), ncol = 2 )
a <- unitweib.reg(y, x)
```

---

Zero adjusted Dirichlet regression

*Zero adjusted Dirichlet regression*

---

**Description**

Zero adjusted Dirichlet regression.

**Usage**

```
zadr(y, x, con = TRUE, B = 1, ncores = 2, xnew = NULL)
zadr2(y, x, con = TRUE, B = 1, ncores = 2, xnew = NULL)
```

**Arguments**

y	A matrix with the compositional data (dependent variable). The number of observations (vectors) with no zero values should be more than the columns of the predictor variables. Otherwise, the initial values will not be calculated.
x	The predictor variable(s), they can be either continuous or categorical or both.
con	If this is TRUE (default) then the constant term is estimated, otherwise the model includes no constant term.
B	If B is greater than 1 bootstrap estimates of the standard error are returned. If you set this greater than 1, then you must define the number of clusters in order to run in parallel.
ncores	The number of cores to use when B>1. This is to be used for the case of bootstrap. If B = 1, this is not taken into consideration. If this does not work then you might need to load the doParallel yourselves.
xnew	If you have new data use it, otherwise leave it NULL.

**Details**

A zero adjusted Dirichlet regression is being fitted. The likelihood consists of two components. The contributions of the non zero compositional values and the contributions of the compositional vectors with at least one zero value. The second component may have many different sub-categories, one for each pattern of zeros. The function "zadr2()" links the covariates to the alpha parameters of the Dirichlet distribution, i.e. it uses the classical parametrization of the distribution. This means, that there is a set of regression parameters for each component.

**Value**

A list including:

runtime	The time required by the regression.
loglik	The value of the log-likelihood.
phi	The precision parameter.
be	The beta coefficients.
seb	The standard error of the beta coefficients.
sigma	The covariance matrix of the regression parameters (for the mean vector and the phi parameter).
est	The fitted or the predicted values (if xnew is not NULL).

**Author(s)**

Michail Tsagris.

R implementation and documentation: Michail Tsagris <mtsagris@uoc.gr>.

**References**

Tsagris M. and Stewart C. (2018). A Dirichlet regression model for compositional data with zeros. *Lobachevskii Journal of Mathematics*,39(3): 398–412.

Preprint available from <https://arxiv.org/pdf/1410.5011.pdf>

**See Also**

[zad.est](#), [diri.reg](#), [kl.compreg](#), [ols.compreg](#), [alfa.reg](#)

**Examples**

```
x <- as.vector(iris[, 4])
y <- as.matrix(iris[, 1:3])
y <- y / rowSums(y)
mod1 <- diri.reg(y, x)
y[sample(1:450, 15) ] <- 0
mod2 <- zadr(y, x)
```

# Index

- \* **Additive log-ratio-transformation**
  - The additive log-ratio transformation and its inverse, [202](#)
- \* **Bhattacharyya distance**
  - Kullback-Leibler divergence and Bhattacharyya distance between two Dirichlet distributions, [109](#)
- \* **Compositional data**
  - Compositional-package, [7](#)
- \* **Contour plots**
  - Compositional-package, [7](#)
- \* **Dirichlet mean vector**
  - Log-likelihood ratio test for a Dirichlet mean vector, [124](#)
- \* **Dirichlet distribution**
  - Contour plot of the Dirichlet distribution in  $S^2$ , [20](#)
  - Contour plot of the Flexible Dirichlet distribution in  $S^2$ , [21](#)
  - Contour plot of the generalised Dirichlet distribution in  $S^2$ , [23](#)
  - Density values of a Dirichlet distribution, [60](#)
  - Density values of a generalised Dirichlet distribution, [61](#)
  - Dirichlet random values simulation, [64](#)
  - Kullback-Leibler divergence and Bhattacharyya distance between two Dirichlet distributions, [109](#)
  - Minimized Kullback-Leibler divergence between Dirichlet and logistic normal, [126](#)
  - MLE of the Dirichlet distribution, [133](#)
  - MLE of the Dirichlet distribution via Newton-Raphson, [134](#)
- \* **Dirichlet regression**
  - Dirichlet regression, [65](#)
- \* **Discriminant analysis**
  - Compositional-package, [7](#)
- \* **Euclidean distance**
  - The alpha-distance, [203](#)
  - The alpha-IT-distance, [206](#)
  - The k-nearest neighbours using the alpha-distance, [220](#)
- \* **Frechet mean**
  - Helper Frechet mean for compositional data, [93](#)
  - The Frechet mean for compositional data, [218](#)
- \* **GLM**
  - Tuning the principal components with GLMs, [246](#)
- \* **Gaussian mixture models**
  - Density of compositional data from Gaussian mixture models, [56](#)
  - Density of the folded normal distribution, [59](#)
  - Simulation of compositional data from Gaussian mixture models, [191](#)
  - Simulation of compositional data from the folded normal distribution, [194](#)
- \* **Gaussianmixture model**
  - Contour plot of the Gaussian mixture model in  $S^2$ , [22](#)
- \* **Generalised Dirichlet distribution**
  - Generalised Dirichlet random values simulation, [90](#)
- \* **Kullback-Leibler divergence**
  - Helper functions for the

- Kullback-Leibler regression, [94](#)
- \* **Kullback-Leibler divergence**
  - Kullback-Leibler divergence and Bhattacharyya distance between two Dirichlet distributions, [109](#)
- \* **Log-likelihood ratio test**
  - Log-likelihood ratio test for a Dirichlet mean vector, [124](#)
  - Log-likelihood ratio test for a symmetric Dirichlet distribution, [125](#)
- \* **MLE**
  - Compositional-package, [7](#)
- \* **Manhattan distance**
  - The alpha-distance, [203](#)
  - The alpha-IT-distance, [206](#)
  - The k-nearest neighbours using the alpha-distance, [220](#)
- \* **Multiplicative log-ratio-transformation**
  - The multiplicative log-ratio transformation and its inverse, [224](#)
- \* **Multivariate analysis of variance**
  - Two-sample test of high-dimensional means for compositional data, [250](#)
- \* **Multivariate hypothesis testing**
  - Exponential empirical likelihood hypothesis testing for two mean vectors, [82](#)
  - Hypothesis testing for two or more compositional mean vectors, [98](#)
- \* **Newton-Raphson**
  - MLE of the Dirichlet distribution via Newton-Raphson, [134](#)
- \* **Regression**
  - Compositional-package, [7](#)
- \* **Regularised discriminant analysis**
  - Cross validation for the regularised and flexible discriminant analysis with compositional data using the alpha-transformation, [36](#)
  - Regularised and flexible discriminant analysis for compositional data using the alpha-transformation, [181](#)
  - Regularised discriminant analysis for Euclidean data, [183](#)
  - Tuning of the k-NN algorithm for compositional data, [236](#)
- \* **Ridge regression**
  - Cross validation for the ridge regression, [38](#)
- \* **Unequality of the covariance matrices**
  - Two-sample test of high-dimensional means for compositional data, [250](#)
- \* **bandwidth tuning**
  - Tuning of the bandwidth  $h$  of the kernel using the maximum likelihood cross validation, [233](#)
- \* **bivariate normal distribution**
  - Contour plot of the alpha multivariate normal in  $S^2$ , [17](#)
  - Contour plot of the alpha-folded model in  $S^2$ , [18](#)
  - Contour plot of the normal distribution in  $S^2$ , [26](#)
- \* **bivariate skew skewnormal distribution**
  - Contour plot of the skew skew-normal distribution in  $S^2$ , [27](#)
- \* **bivariate t distribution**
  - Contour plot of the t distribution in  $S^2$ , [28](#)
- \* **compositional data**
  - Hypothesis testing for two or more compositional mean vectors, [98](#)
- \* **contour plot**
  - Contour plot of the alpha multivariate normal in  $S^2$ , [17](#)
  - Contour plot of the alpha-folded model in  $S^2$ , [18](#)
  - Contour plot of the Dirichlet distribution in  $S^2$ , [20](#)
  - Contour plot of the Flexible Dirichlet distribution in  $S^2$ , [21](#)
  - Contour plot of the Gaussian mixture model in  $S^2$ , [22](#)
  - Contour plot of the generalised Dirichlet distribution in  $S^2$ ,



- 23
- Contour plot of the kernel density estimate in  $S^2$ , 24
- Contour plot of the normal distribution in  $S^2$ , 26
- Contour plot of the skew skew-normal distribution in  $S^2$ , 27
- Contour plot of the t distribution in  $S^2$ , 28
- \* **cross-validation**
  - Cross validation for the regularised and flexible discriminant analysis with compositional data using the alpha-transformation, 36
- \* **density values**
  - Density values of a Dirichlet distribution, 60
  - Density values of a generalised Dirichlet distribution, 61
- \* **inverse transformation**
  - Inverse of the alpha-transformation, 105
- \* **kernel density estimate**
  - Multivariate kernel density estimation, 140
- \* **kernel density**
  - Contour plot of the kernel density estimate in  $S^2$ , 24
  - Tuning of the bandwidth  $h$  of the kernel using the maximum likelihood cross validation, 233
- \* **location and scatter**
  - Estimating location and scatter parameters for compositional data, 77
- \* **maximum likelihood cross validation**
  - Tuning of the bandwidth  $h$  of the kernel using the maximum likelihood cross validation, 233
- \* **maximum likelihood estimation**
  - Estimation of the value of alpha in the folded model, 80
  - Minimized Kullback-Leibler divergence between Dirichlet and logistic normal, 126
  - MLE of the Dirichlet distribution, 133
  - MLE of the Dirichlet distribution via Newton-Raphson, 134
  - MLE of the folded model for a given value of alpha, 135
- \* **maximum log-likelihood estimation**
  - Fast estimation of the value of alpha, 85
- \* **mixtures of normal distributions**
  - Mixture model selection via BIC, 127
- \* **model selection**
  - Mixture model selection via BIC, 127
- \* **multivariate kernel**
  - Multivariate kernel density estimation, 140
- \* **multivariate linear regression**
  - Multivariate linear regression, 143
- \* **multivariate normal distribution**
  - Multivariate normal random values simulation on the simplex, 144
- \* **multivariate regression**
  - Dirichlet regression, 65
  - Helper functions for the Kullback-Leibler regression, 94
  - Non linear least squares regression for compositional data, 154
  - Spatial median regression, 195
- \* **multivariate regression**
  - Multivariate regression with compositional data, 147
- \* **multivariate skew normal distribution**
  - Multivariate skew normal random values simulation on the simplex, 148
- \* **multivariate t distribution**
  - MLE for the multivariate t distribution, 130
  - Multivariate t random values simulation on the simplex, 150
- \* **non parametric test**
  - Exponential empirical likelihood hypothesis testing for two

- mean vectors, [82](#)
    - Hypothesis testing for two or more compositional mean vectors, [98](#)
  - \* **ordinary least squares**
    - Non linear least squares regression for compositional data, [154](#)
  - \* **orthogonal matrix**
    - The Helmert sub-matrix, [219](#)
  - \* **parameters tuning**
    - Cross validation for the ridge regression with compositional data as predictor using the alpha-transformation, [40](#)
  - \* **plot**
    - Ridge regression plot, [185](#)
    - Ridge regression with the alpha-transformation plot, [188](#)
  - \* **principal components regression**
    - Multivariate or univariate regression with compositional data in the covariates side using the alpha-transformation, [145](#)
    - Tuning the number of PCs in the PCR with compositional data using the alpha-transformation, [243](#)
  - \* **principal components**
    - Tuning the principal components with GLMs, [246](#)
  - \* **profile log-likelihood**
    - Estimation of the value of alpha via the profile log-likelihood, [81](#)
  - \* **random values simulation**
    - Dirichlet random values simulation, [64](#)
    - Generalised Dirichlet random values simulation, [90](#)
    - Multivariate normal random values simulation on the simplex, [144](#)
    - Multivariate skew normal random values simulation on the simplex, [148](#)
    - Multivariate t random values simulation on the simplex, [150](#)
  - \* **random vectors simulation**
    - Density of compositional data from Gaussian mixture models, [56](#)
    - Density of the folded normal distribution, [59](#)
    - Simulation of compositional data from Gaussian mixture models, [191](#)
    - Simulation of compositional data from the folded normal distribution, [194](#)
  - \* **ridge regression**
    - Cross validation for the ridge regression with compositional data as predictor using the alpha-transformation, [40](#)
    - Ridge regression plot, [185](#)
    - Ridge regression with compositional data in the covariates side using the alpha-transformation, [187](#)
    - Ridge regression with the alpha-transformation plot, [188](#)
  - \* **robust estimation**
    - Estimating location and scatter parameters for compositional data, [77](#)
  - \* **spatial median regression**
    - Multivariate regression with compositional data, [147](#)
    - Spatial median regression, [195](#)
  - \* **symmetric Dirichlet distribution**
    - Log-likelihood ratio test for a symmetric Dirichlet distribution, [125](#)
  - \* **ternary plot**
    - Ternary diagram, [196](#)
    - Ternary diagram of regression models, [198](#)
  - \* **tuning**
    - Tuning the number of PCs in the PCR with compositional data using the alpha-transformation, [243](#)
  - \* **visualisation**
    - Ternary diagram, [196](#)
    - Ternary diagram of regression models, [198](#)
- a. est, [60](#), [79](#), [136](#), [195](#), [214](#)

- [a.est](#) (Estimation of the value of alpha in the folded model), 80  
[a.mle](#), 214  
[a.mle](#) (MLE of the folded model for a given value of alpha), 135  
[acor](#), 77, 175, 233  
[acor](#) (Alpha-generalised correlations between two compositional datasets), 10  
[acor.tune](#), 11, 77  
[acor.tune](#) (Tuning of the alpha-generalised correlations between two compositional datasets), 232  
[aeqdist.etest](#), 11  
[aeqdist.etest](#) (Energy test of equality of distributions using the alpha-transformation), 76  
[ait](#), 207  
[ait](#) (The alpha-IT transformation), 205  
[ait.knn](#), 205  
[ait.knn](#) (The k-NN algorithm for compositional data), 222  
[ait.test](#) (Aitchison's test for two mean vectors and/or covariance matrices), 8  
Aitchison's test for two mean vectors and/or covariance matrices, 8  
[aitdist](#), 205  
[aitdist](#) (The alpha-IT-distance), 206  
[aitdista](#) (The alpha-IT-distance), 206  
[aitknn.tune](#) (Tuning of the k-NN algorithm for compositional data), 236  
[akern.reg](#), 33, 35, 109, 171, 208  
[akern.reg](#) (The alpha-kernel regression with compositional response data), 210  
[akernreg.tune](#), 33, 211, 240  
[akernreg.tune](#) (Cross validation for the alpha-kernel regression with compositional response data), 33  
[aknn.reg](#), 33, 35, 36, 93, 109, 171, 209, 211  
[aknn.reg](#) (The alpha-k-NN regression for compositional response data), 207  
[aknnreg.tune](#), 30, 35, 36, 208, 211, 240  
[aknnreg.tune](#) (Cross validation for the alpha-k-NN regression with compositional response data), 32  
[alef](#) (The alpha-transformation), 213  
[alfa](#), 10, 11, 77, 79, 81, 82, 86, 89, 92, 94, 106, 130, 136, 156, 164, 182, 195, 203–205, 207, 216, 218–221, 223–225, 232, 233, 244, 249  
[alfa](#) (The alpha-transformation), 213  
[alfa.contour](#), 19  
[alfa.contour](#) (Contour plot of the alpha multivariate normal in  $S^2$ ), 17  
[alfa.fda](#), 31, 33, 35  
[alfa.fda](#) (Regularised and flexible discriminant analysis for compositional data using the alpha-transformation), 181  
[alfa.knn](#), 64, 87, 89, 130, 152, 153, 182, 209, 221  
[alfa.knn](#) (The k-NN algorithm for compositional data), 222  
[alfa.knn.reg](#), 13, 44, 111, 114, 122, 123, 253, 255  
[alfa.knn.reg](#) (The alpha-k-NN regression with compositional predictor variables), 208  
[alfa.lasso](#), 44  
[alfa.lasso](#) (LASSO with compositional predictors using the alpha-transformation), 113  
[alfa.mds](#), 170  
[alfa.mds](#) (Principal coordinate analysis using the alpha-distance), 168  
[alfa.mix.norm](#), 87, 130  
[alfa.mix.norm](#) (Gaussian mixture models for compositional data using the alpha-transformation), 88  
[alfa.nb](#), 53, 182, 221, 223  
[alfa.nb](#) (Naive Bayes classifiers for compositional data using the alpha-transformation), 152  
[alfa.pca](#), 165, 169, 170  
[alfa.pca](#) (Principal component analysis using the alpha-transformation), 165  
[alfa.pcr](#), 13, 100, 104, 111, 122, 123,

- 165–167, 172, 209, 244, 248, 253, 255
- alfa.pcr (Multivariate or univariate regression with compositional data in the covariates side using the alpha-transformation), 145
- alfa.pprcomp, 242
- alfa.pprcomp (Projection pursuit regression with compositional predictor variables using the alpha-transformation), 172
- alfa.profile, 11, 77, 81, 85, 86, 136, 214, 232, 233
- alfa.profile (Estimation of the value of alpha via the profile log-likelihood), 81
- alfa.rda, 31, 33, 35, 38, 64, 87, 89, 130, 152, 153, 221, 223
- alfa.rda (Regularised and flexible discriminant analysis for compositional data using the alpha-transformation), 181
- alfa.reg, 67, 155, 171, 196, 204, 208, 211, 249, 262
- alfa.reg (Regression with compositional data using the alpha-transformation), 179
- alfa.reg2 (Regression with compositional data using the alpha-transformation), 179
- alfa.reg3 (Regression with compositional data using the alpha-transformation), 179
- alfa.ridge, 41, 185, 186, 189, 209
- alfa.ridge (Ridge regression with compositional data in the covariates side using the alpha-transformation), 187
- alfa.tune, 82, 214, 232
- alfa.tune (Fast estimation of the value of alpha), 85
- alfadist, 106, 207, 217
- alfadist (The alpha-distance), 203
- alfadista (The alpha-distance), 203
- alfafda.tune (Cross validation for the regularised and flexible discriminant analysis with compositional data using the alpha-transformation), 36
- alfainv, 81, 82, 86, 94, 136, 203, 204, 214, 219–221, 225, 233
- alfainv (Inverse of the alpha-transformation), 105
- alfaknn.tune (Tuning of the k-NN algorithm for compositional data), 236
- alfaknnreg.tune (Cross validation for the alpha-k-NN regression with compositional predictor variables), 30
- alfalasso.tune, 114
- alfalasso.tune (Cross-validation for LASSO with compositional predictors using the alpha-transformation), 43
- alfanb.tune, 38, 48
- alfanb.tune (Cross-validation for the naive Bayes classifiers for compositional data using the alpha-transformation), 52
- alfann (The k-nearest neighbours using the alpha-distance), 220
- alfapcr.tune, 72, 147, 167, 236, 241, 247, 248
- alfapcr.tune (Tuning the number of PCs in the PCR with compositional data using the alpha-transformation), 243
- alfapprcomp.tune, 173
- alfapprcomp.tune (Tuning of the projection pursuit regression with compositional predictor variables using the alpha-transformation), 241
- alfarda.tune, 48, 53, 182, 238
- alfarda.tune (Cross validation for the regularised and flexible discriminant analysis with compositional data using the alpha-transformation), 36
- alfareg.tune, 147, 180, 181
- alfareg.tune (Tuning the value of alpha in the alpha-regression), 248
- alfaridge.plot, 186, 188
- alfaridge.plot (Ridge regression with

- the alpha-transformation plot), 188
- alfaridge.tune, 39, 188
- alfaridge.tune (Cross validation for the ridge regression with compositional data as predictor using the alpha-transformation), 40
- All pairwise additive log-ratio transformations, 9
- Alpha-generalised correlations between two compositional datasets, 10
- alpha.mle, 79, 81, 195, 214
- alpha.mle (MLE of the folded model for a given value of alpha), 135
- alr, 10, 50, 112, 175, 205, 214–218, 224, 225
- alr (The additive log-ratio transformation and its inverse), 202
- alr.all (All pairwise additive log-ratio transformations), 9
- alrinv (The additive log-ratio transformation and its inverse), 202
- ANOVA for the log-contrast GLM versus the unconstrained GLM, 12
- ANOVA for the log-contrast regression versus the unconstrained linear regression, 13
- ascls, 46, 213
- ascls (The alpha-SCLS model), 211
- atflr, 47, 212
- atflr (The alpha-TFLR model), 212
- bc, 203, 214, 218
- bc (The Box-Cox transformation applied to ratios of components), 215
- Beta regression, 14
- beta.est, 14, 16, 178
- beta.est (MLE of distributions defined in the  $(0, 1)$  interval), 131
- beta.reg, 68, 177, 261
- beta.reg (Beta regression), 14
- bic.alfamixnorm, 89, 128
- bic.alfamixnorm (Mixture model selection with the alpha-transformation using BIC), 128
- bic.mixcompnorm, 23, 57, 87, 89, 191
- bic.mixcompnorm (Mixture model selection via BIC), 127
- bivt.contour, 18, 19, 22, 25, 26, 28, 130, 131
- bivt.contour (Contour plot of the  $t$  distribution in  $S^2$ ), 28
- colbeta.est, 178
- colbeta.est (Column-wise MLE of some univariate distributions), 15
- collogitnorm.est (Column-wise MLE of some univariate distributions), 15
- Column-wise MLE of some univariate distributions, 15
- colunitweibull.est (Column-wise MLE of some univariate distributions), 15
- colzilogitnorm.est (Column-wise MLE of some univariate distributions), 15
- comp.den, 130, 131, 145, 149, 150
- comp.den (Estimating location and scatter parameters for compositional data), 77
- comp.kern (Multivariate kernel density estimation for compositional data), 142
- comp.kerncontour, 17, 20, 22, 24, 141, 143, 234
- comp.kerncontour (Contour plot of the kernel density estimate in  $S^2$ ), 24
- comp.knn, 64, 73, 152, 153, 217, 238
- comp.knn (The  $k$ -NN algorithm for compositional data), 222
- comp.nb, 52, 64, 87, 89, 130, 153, 182, 221, 223
- comp.nb (Naive Bayes classifiers for compositional data), 151
- comp.ppr, 100, 172, 173, 208, 211, 240
- comp.ppr (Projection pursuit regression for compositional data), 170
- comp.reg, 30, 51, 67, 70, 95, 113, 144, 155, 163, 171, 181, 196, 208, 211
- comp.reg (Multivariate regression with compositional data), 147
- comp.test, 9, 174, 250

- comp.test (Hypothesis testing for two or more compositional mean vectors), [98](#)
- compknn.tune, [38](#), [48](#), [53](#), [91](#), [223](#)
- compknn.tune (Tuning of the k-NN algorithm for compositional data), [236](#)
- compnorm.contour, [17–20](#), [22](#), [24](#), [25](#), [28](#), [29](#)
- compnorm.contour (Contour plot of the normal distribution in  $S^2$ ), [26](#)
- Compositional-package, [7](#)
- compmpr.tune, [30](#), [171](#), [241](#), [242](#)
- compmpr.tune (Tuning of the projection pursuit regression for compositional data), [239](#)
- Contour plot of mixtures of Dirichlet distributions in  $S^2$ , [16](#)
- Contour plot of the alpha multivariate normal in  $S^2$ , [17](#)
- Contour plot of the alpha-folded model in  $S^2$ , [18](#)
- Contour plot of the Dirichlet distribution in  $S^2$ , [20](#)
- Contour plot of the Flexible Dirichlet distribution in  $S^2$ , [21](#)
- Contour plot of the Gaussian mixture model in  $S^2$ , [22](#)
- Contour plot of the generalised Dirichlet distribution in  $S^2$ , [23](#)
- Contour plot of the kernel density estimate in  $S^2$ , [24](#)
- Contour plot of the normal distribution in  $S^2$ , [26](#)
- Contour plot of the skew skew-normal distribution in  $S^2$ , [27](#)
- Contour plot of the t distribution in  $S^2$ , [28](#)
- Cross validation for some compositional regression models, [29](#)
- Cross validation for the alpha-k-NN regression with compositional predictor variables, [30](#)
- Cross validation for the alpha-k-NN regression with compositional response data, [32](#)
- Cross validation for the alpha-kernel regression with compositional response data, [33](#)
- Cross validation for the kernel regression with Euclidean response data, [35](#)
- Cross validation for the regularised and flexible discriminant analysis with compositional data using the alpha-transformation, [36](#)
- Cross validation for the ridge regression, [38](#)
- Cross validation for the ridge regression with compositional data as predictor using the alpha-transformation, [40](#)
- Cross validation for the TFLR model, [42](#)
- Cross-validation for LASSO with compositional predictors using the alpha-transformation, [43](#)
- Cross-validation for the alpha-SCLS model, [45](#)
- Cross-validation for the alpha-TFLR model, [46](#)
- Cross-validation for the Dirichlet discriminant analysis, [47](#)
- Cross-validation for the LASSO Kullback-Leibler divergence based regression, [48](#)
- Cross-validation for the LASSO log-ratio regression with compositional response, [50](#)
- Cross-validation for the naive Bayes classifiers for compositional data, [51](#)
- Cross-validation for the naive Bayes classifiers for compositional data using the alpha-transformation, [52](#)
- Cross-validation for the SCLS model, [54](#)
- Cross-validation for the SCRQ model, [55](#)
- cv.ascls, [47](#), [212](#)
- cv.ascls (Cross-validation for the alpha-SCLS model), [45](#)
- cv.atflr, [46](#), [213](#)
- cv.atflr (Cross-validation for the alpha-TFLR model), [46](#)
- cv.comp.reg (Cross validation for some

- compositional regression models), 29
- cv.compnb, 38, 48, 53, 152, 238
- cv.compnb (Cross-validation for the naive Bayes classifiers for compositional data), 51
- cv.dda, 38, 53, 64, 238
- cv.dda (Cross-validation for the Dirichlet discriminant analysis), 47
- cv.lasso.compreg, 49, 113, 163
- cv.lasso.compreg (Cross-validation for the LASSO log-ratio regression with compositional response), 50
- cv.lasso.klcompreg, 44, 51, 111, 113, 114, 163
- cv.lasso.klcompreg (Cross-validation for the LASSO Kullback-Leibler divergence based regression), 48
- cv.scls, 43, 56, 227–229
- cv.scls (Cross-validation for the SCLS model), 54
- cv.scrq (Cross-validation for the SCRQ model), 55
- cv.tflr, 55, 56, 231, 236
- cv.tflr (Cross validation for the TFLR model), 42
  
- dda, 17, 48, 61, 62, 67, 127, 134, 135, 152
- dda (Dirichlet discriminant analysis), 63
- ddiri, 62, 125, 127, 134, 135
- ddiri (Density values of a Dirichlet distribution), 60
- Density of compositional data from Gaussian mixture models, 56
- Density of the Flexible Dirichlet distribution, 58
- Density of the folded normal distribution, 59
- Density values of a Dirichlet distribution, 60
- Density values of a generalised Dirichlet distribution, 61
- Density values of a mixture of Dirichlet distributions, 62
- dfd, 194
- dfd (Density of the Flexible Dirichlet distribution), 58
- dfolded (Density of the folded normal distribution), 59
- dgendiri, 61
- dgendiri (Density values of a generalised Dirichlet distribution), 61
- diri.contour, 17–19, 23–26, 28, 29, 61, 62, 65, 91, 127, 134, 135, 197, 198, 201
- diri.contour (Contour plot of the Dirichlet distribution in  $S^2$ ), 20
- diri.est, 8, 61, 62, 65, 91, 110, 125, 126, 132, 135
- diri.est (MLE of the Dirichlet distribution), 133
- diri.nr, 17, 61, 65, 67, 91, 110, 125–127, 134, 137
- diri.nr (MLE of the Dirichlet distribution via Newton-Rapshon), 134
- diri.reg, 7, 8, 14, 64, 70, 95, 127, 134, 144, 148, 155, 181, 196, 262
- diri.reg (Dirichlet regression), 65
- diri.reg2 (Dirichlet regression), 65
- diri.reg3 (Dirichlet regression), 65
- Dirichlet discriminant analysis, 63
- Dirichlet random values simulation, 64
- Dirichlet regression, 65
- dirimean.test, 8, 126
- dirimean.test (Log-likelihood ratio test for a Dirichlet mean vector), 124
- Distance based regression models for proportions, 67
- divergence (Divergence matrix of compositional data), 73
- Divergence based regression for compositional data, 69
- Divergence based regression for compositional data with compositional data in the covariates side using the alpha-transformation, 71
- Divergence matrix of compositional data, 73
- dmix.compnorm (Density of

- compositional data from Gaussian mixture models), 56
- dmixdiri (Density values of a mixture of Dirichlet distributions), 62
- dptest, 99
- dptest (Projections based test for distributional equality of two groups), 174
- eel.test2, 75, 97, 108
- eel.test2 (Exponential empirical likelihood hypothesis testing for two mean vectors), 82
- el.test2, 84, 97, 108
- el.test2 (Empirical likelihood hypothesis testing for two mean vectors), 74
- Empirical likelihood hypothesis testing for two mean vectors, 74
- Energy test of equality of distributions using the alpha-transformation, 76
- es (The ESOV-distance), 216
- esov, 204, 223
- esov (The ESOV-distance), 216
- esov.mds, 169
- esov.mds (Principal coordinate analysis using the Jensen-Shannon divergence), 169
- esova (The ESOV-distance), 216
- Estimating location and scatter parameters for compositional data, 77
- Estimation of the probability left outside the simplex when using the alpha-transformation, 78
- Estimation of the value of alpha in the folded model, 80
- Estimation of the value of alpha via the profile log-likelihood, 81
- Exponential empirical likelihood hypothesis testing for two mean vectors, 82
- Fast estimation of the value of alpha, 85
- fd.contour (Contour plot of the Flexible Dirichlet distribution in  $S^2$ ), 21
- folded.contour, 18, 22, 60
- folded.contour (Contour plot of the alpha-folded model in  $S^2$ ), 18
- fp, 203, 214, 216
- fp (The folded power transformation), 217
- frechet (The Frechet mean for compositional data), 218
- frechet2 (Helper Frechet mean for compositional data), 93
- Gaussian mixture models for compositional data, 86
- Gaussian mixture models for compositional data using the alpha-transformation, 88
- gendiri.contour, 17, 20
- gendiri.contour (Contour plot of the generalised Dirichlet distribution in  $S^2$ ), 23
- Generalised Dirichlet random values simulation, 90
- Generate random folds for cross-validation, 91
- glm, 244
- glm.pcr, 72, 147, 236, 248
- glm.pcr (Principal component generalised linear models), 166
- glmprcr.tune, 244
- glmprcr.tune (Tuning the principal components with GLMs), 246
- green, 203, 205, 214, 216, 218, 224, 225
- green (Greenacre's power transformation), 92
- Greenacre's power transformation, 92
- hd.meantest2, 99
- hd.meantest2 (Two-sample test of high-dimensional means for compositional data), 250
- helling.prop.reg (Distance based regression models for proportions), 67
- hellinger.compreg (Divergence based regression for compositional data), 69
- helm (The Helmert sub-matrix), 219



- Helper Frechet mean for compositional data, [93](#)
- Helper functions for the Kullback-Leibler regression, [94](#)
- hotel2T2, [75](#), [84](#), [106](#), [108](#), [139](#), [140](#)
- hotel2T2 (Hotelling's multivariate version of the 2 sample t-test for Euclidean data), [96](#)
- Hotelling's multivariate version of the 2 sample t-test for Euclidean data, [96](#)
- hsecant01.est (MLE of distributions defined in the  $(0, 1)$  interval), [131](#)
- Hypothesis testing for two or more compositional mean vectors, [98](#)
- ibeta.est (MLE of distributions defined in the  $(0, 1)$  interval), [131](#)
- ICE plot for projection pursuit regression with compositional predictor variables, [99](#)
- ICE plot for the alpha-k-NN regression, [101](#)
- ICE plot for the alpha-kernel regression, [102](#)
- ICE plot for univariate kernel regression, [103](#)
- ice.akernreg, [102](#)
- ice.akernreg (ICE plot for the alpha-kernel regression), [102](#)
- ice.aknnreg, [103](#)
- ice.aknnreg (ICE plot for the alpha-k-NN regression), [101](#)
- ice.kernreg, [100](#), [109](#)
- ice.kernreg (ICE plot for univariate kernel regression), [103](#)
- ice.pprcomp, [102–104](#), [172](#), [241](#)
- ice.pprcomp (ICE plot for projection pursuit regression with compositional predictor variables), [99](#)
- Inverse of the alpha-transformation, [105](#)
- james, [75](#), [84](#), [97](#), [139](#), [140](#)
- james (James multivariate version of the t-test), [106](#)
- James multivariate version of the t-test, [106](#)
- js.compreg, [7](#), [67](#), [73](#), [95](#), [144](#), [148](#), [155](#), [181](#), [196](#), [217](#)
- js.compreg (Divergence based regression for compositional data), [69](#)
- kern.reg, [36](#)
- kern.reg (Kernel regression with a numerical response vector or matrix), [108](#)
- Kernel regression with a numerical response vector or matrix, [108](#)
- kernreg.tune, [104](#), [109](#)
- kernreg.tune (Cross validation for the kernel regression with Euclidean response data), [35](#)
- kl.alfapcr, [165](#), [166](#), [231](#), [236](#)
- kl.alfapcr (Divergence based regression for compositional data with compositional data in the covariates side using the alpha-transformation), [71](#)
- kl.compreg, [8](#), [30](#), [49](#), [67](#), [95](#), [111](#), [144](#), [155](#), [163](#), [171](#), [181](#), [208](#), [211](#), [262](#)
- kl.compreg (Divergence based regression for compositional data), [69](#)
- kl.compreg2 (Helper functions for the Kullback-Leibler regression), [94](#)
- kl.diri (Kullback-Leibler divergence and Bhattacharyya distance between two Dirichlet distributions), [109](#)
- kl.diri.normal (Minimized Kullback-Leibler divergence between Dirichlet and logistic normal), [126](#)
- klalfapcr.tune, [43](#), [55](#), [72](#)
- klalfapcr.tune (Tuning of the divergence based regression for compositional data with compositional data in the covariates side using the alpha-transformation), [235](#)
- klcompreg.boot (Helper functions for the Kullback-Leibler

- regression), 94
- Kullback-Leibler divergence and Bhattacharyya distance between two Dirichlet distributions, 109
- kumar.est (MLE of distributions defined in the  $(0, 1)$  interval), 131
- LASSO Kullback-Leibler divergence based regression, 110
- LASSO log-ratio regression with compositional response, 112
- LASSO with compositional predictors using the alpha-transformation, 113
- lasso.compreg, 44, 49, 51, 111, 114, 163
- lasso.compreg (LASSO log-ratio regression with compositional response), 112
- lasso.klcompreg, 49, 51, 113, 163
- lasso.klcompreg (LASSO Kullback-Leibler divergence based regression), 110
- lassocoeff.plot, 49, 51, 111, 113
- lassocoeff.plot (Plot of the LASSO coefficients), 162
- lc.glm, 8, 12, 117, 251, 252, 256, 258
- lc.glm (Log-contrast GLMs with compositional predictor variables), 115
- lc.glm2, 116, 252, 256, 258
- lc.glm2 (Log-contrast logistic or Poisson regression with with multiple compositional predictors), 116
- lc.reg, 13, 100, 104, 123, 172, 253, 255
- lc.reg (Log-contrast regression with compositional predictor variables), 121
- lc.reg2, 122, 253–255
- lc.reg2 (Log-contrast regression with multiple compositional predictors), 122
- lc.rq, 120, 257, 259
- lc.rq (Log-contrast quantile regression with compositional predictor variables), 118
- lc.rq2, 119, 259
- lc.rq2 (Log-contrast quantile regression with with multiple compositional predictors), 119
- lclm.aov, 116, 252, 258
- lclm.aov (ANOVA for the log-contrast GLM versus the unconstrained GLM), 12
- lcreg.aov, 122, 123, 253
- lcreg.aov (ANOVA for the log-contrast regression versus the unconstrained linear regression), 13
- lm, 143
- Log-contrast GLMs with compositional predictor variables, 115
- Log-contrast logistic or Poisson regression with with multiple compositional predictors, 116
- Log-contrast quantile regression with compositional predictor variables, 118
- Log-contrast quantile regression with with multiple compositional predictors, 119
- Log-contrast regression with compositional predictor variables, 121
- Log-contrast regression with multiple compositional predictors, 122
- Log-likelihood ratio test for a Dirichlet mean vector, 124
- Log-likelihood ratio test for a symmetric Dirichlet distribution, 125
- logitnorm.est (MLE of distributions defined in the  $(0, 1)$  interval), 131
- logpca, 166
- logpca (Principal component analysis), 164
- makefolds (Generate random folds for cross-validation), 91
- manova, 97
- maov (Multivariate analysis of variance assuming equality of the covariance matrices), 139
- maovjames, 75, 84, 108, 140

- maovjames (Multivariate analysis of variance (James test)), 138  
 Minimized Kullback-Leibler divergence between Dirichlet and logistic normal, 126  
 mix.compnorm, 22, 23, 57, 64, 89, 128, 130, 152, 153, 182, 191, 223  
 mix.compnorm (Gaussian mixture models for compositional data), 86  
 mix.compnorm.contour, 17–20, 22, 24–26, 28, 29, 87, 89, 128, 130  
 mix.compnorm.contour (Contour plot of the Gaussian mixture model in  $S^2$ ), 22  
 mixdiri.contour, 20, 24, 63, 193  
 mixdiri.contour (Contour plot of mixtures of Dirichlet distributions in  $S^2$ ), 16  
 Mixture model selection via BIC, 127  
 Mixture model selection with the alpha-transformation using BIC, 128  
 mkde, 7, 143, 234  
 mkde (Multivariate kernel density estimation), 140  
 mkde.tune, 141  
 mkde.tune (Tuning of the bandwidth  $h$  of the kernel using the maximum likelihood cross validation), 233  
 MLE for the multivariate  $t$  distribution, 130  
 MLE of distributions defined in the  $(0, 1)$  interval, 131  
 MLE of the Dirichlet distribution, 133  
 MLE of the Dirichlet distribution via Newton-Raphson, 134  
 MLE of the folded model for a given value of alpha, 135  
 MLE of the zero adjusted Dirichlet distribution, 137  
 mlr (The multiplicative log-ratio transformation and its inverse), 224  
 mlrinv (The multiplicative log-ratio transformation and its inverse), 224  
 multinompcr.tune (Tuning the principal components with GLMs), 246  
 Multivariate analysis of variance (James test), 138  
 Multivariate analysis of variance assuming equality of the covariance matrices, 139  
 Multivariate kernel density estimation, 140  
 Multivariate kernel density estimation for compositional data, 142  
 Multivariate linear regression, 143  
 Multivariate normal random values simulation on the simplex, 144  
 Multivariate or univariate regression with compositional data in the covariates side using the alpha-transformation, 145  
 Multivariate regression with compositional data, 147  
 Multivariate skew normal random values simulation on the simplex, 148  
 Multivariate  $t$  random values simulation on the simplex, 150  
 multivreg, 148, 196  
 multivreg (Multivariate linear regression), 143  
 multivt, 78  
 multivt (MLE for the multivariate  $t$  distribution), 130  
 Naive Bayes classifiers for compositional data, 151  
 Naive Bayes classifiers for compositional data using the alpha-transformation, 152  
 Non linear least squares regression for compositional data, 154  
 Non-parametric zero replacement strategies, 155  
 ols.compreg, 67, 70, 95, 111, 144, 177, 181, 262  
 ols.compreg (Non linear least squares regression for compositional data), 154  
 ols.prop.reg (Distance based regression models for proportions), 67  
 optim, 226, 227

- optimize, [180](#)
- pcc (Proportionality correlation coefficient matrix), [175](#)
- pcr.tune, [244](#), [248](#)
- pcr.tune (Tuning the principal components with GLMs), [246](#)
- Permutation linear independence test in the SCLS model, [156](#)
- Permutation linear independence test in the TFLR model, [157](#)
- Permutation test for the matrix of coefficients in the SCLS model, [158](#)
- Permutation test for the matrix of coefficients in the TFLR model, [160](#)
- perturbation, [156](#), [164](#)
- perturbation (Perturbation operation), [161](#)
- Perturbation operation, [161](#)
- pivot, [203](#), [214](#), [224](#)
- pivot (The pivot coordinate transformation and its inverse), [225](#)
- pivotinv (The pivot coordinate transformation and its inverse), [225](#)
- Plot of the LASSO coefficients, [162](#)
- pow (Power operation), [163](#)
- power, [162](#)
- Power operation, [163](#)
- pprcomp, [100](#), [173](#), [241](#)
- pprcomp (Projection pursuit regression with compositional predictor variables), [171](#)
- pprcomp.tune, [100](#), [172](#), [242](#)
- pprcomp.tune (Tuning of the projection pursuit regression with compositional predictor variables), [240](#)
- Principal component analysis, [164](#)
- Principal component analysis using the alpha-transformation, [165](#)
- Principal component generalised linear models, [166](#)
- Principal coordinate analysis using the alpha-distance, [168](#)
- Principal coordinate analysis using the Jensen-Shannon divergence, [169](#)
- probout (Estimation of the probability left outside the simplex when using the alpha-transformation), [78](#)
- profile, [94](#), [219](#), [244](#)
- Projection pursuit regression for compositional data, [170](#)
- Projection pursuit regression with compositional predictor variables, [171](#)
- Projection pursuit regression with compositional predictor variables using the alpha-transformation, [172](#)
- Projections based test for distributional equality of two groups, [174](#)
- Proportionality correlation coefficient matrix, [175](#)
- propreg, [14](#), [68](#), [261](#)
- propreg (Quasi binomial regression for proportions), [176](#)
- propregs (Quasi binomial regression for proportions), [176](#)
- Quasi binomial regression for proportions, [176](#)
- Random values generation from some univariate distributions defined on the  $(0,1)$  interval, [177](#)
- rbeta1 (Random values generation from some univariate distributions defined on the  $(0,1)$  interval), [177](#)
- rcompnorm, [149](#), [150](#)
- rcompnorm (Multivariate normal random values simulation on the simplex), [144](#)
- rcompsn, [145](#)
- rcompsn (Multivariate skew normal random values simulation on the simplex), [148](#)
- rcompt, [145](#)

- rcompt (Multivariate t random values simulation on the simplex), 150
- rda, 246
- rda (Regularised discriminant analysis for Euclidean data), 183
- rda.tune, 184
- rda.tune (Tuning the parameters of the regularised discriminant analysis), 245
- rdiri, 61, 62, 90, 91, 125–127, 134, 135, 145, 149, 150, 178
- rdiri (Dirichlet random values simulation), 64
- Read a file as a Filebacked Big Matrix, 178
- read.fbm (Read a file as a Filebacked Big Matrix), 178
- Regression with compositional data using the alpha-transformation, 179
- Regularised and flexible discriminant analysis for compositional data using the alpha-transformation, 181
- Regularised discriminant analysis for Euclidean data, 183
- rfd, 58
- rfd (Simulation of compositional data from the Flexible Dirichlet distribution), 193
- rfolded, 60, 79
- rfolded (Simulation of compositional data from the folded normal distribution), 194
- rgendiri, 62, 65
- rgendiri (Generalised Dirichlet random values simulation), 90
- Ridge regression, 184
- Ridge regression plot, 185
- Ridge regression with compositional data in the covariates side using the alpha-transformation, 187
- Ridge regression with the alpha-transformation plot, 188
- ridge.plot, 185, 189
- ridge.plot (Ridge regression plot), 185
- ridge.reg, 39, 186–188
- ridge.reg (Ridge regression), 184
- ridge.tune, 41, 185, 186
- ridge.tune (Cross validation for the ridge regression), 38
- rlogitnorm (Random values generation from some univariate distributions defined on the  $(0,1)$  interval), 177
- rmixcomp, 87, 89, 128, 130, 193
- rmixcomp (Simulation of compositional data from Gaussian mixture models), 191
- rmixdiri, 63
- rmixdiri (Simulation of compositional data from mixtures of Dirichlet distributions), 192
- runitweibull (Random values generation from some univariate distributions defined on the  $(0,1)$  interval), 177
- scls, 55, 156–159, 161, 179, 190, 200–202, 212, 231
- scls (The SCLS model), 226
- scls.betest, 157
- scls.betest (Permutation test for the matrix of coefficients in the SCLS model), 158
- scls.indeptest, 159, 161, 227–229
- scls.indeptest (Permutation linear independence test in the SCLS model), 156
- scls2, 157, 159
- scls2 (The SCLS model with multiple compositional predictors), 227
- scrq, 56, 227
- scrq (Simplicial constrained median regression for compositional responses and predictors model), 189
- Simplicial constrained median regression for compositional responses and predictors model, 189
- Simulation of compositional data from Gaussian mixture models, 191
- Simulation of compositional data from mixtures of Dirichlet distributions, 192

- Simulation of compositional data from the Flexible Dirichlet distribution, [193](#)
- Simulation of compositional data from the folded normal distribution, [194](#)
- skewnorm.contour, [18](#), [19](#), [26](#), [29](#)
- skewnorm.contour (Contour plot of the skew skew-normal distribution in  $S^2$ ), [27](#)
- Spatial median regression, [195](#)
- spatmed.reg, [78](#), [148](#)
- spatmed.reg (Spatial median regression), [195](#)
- sym.test, [125](#)
- sym.test (Log-likelihood ratio test for a symmetric Dirichlet distribution), [125](#)
- symkl.compreg (Divergence based regression for compositional data), [69](#)
- ternary, [198](#), [200–202](#)
- ternary (Ternary diagram), [196](#)
- Ternary diagram, [196](#)
- Ternary diagram of regression models, [198](#)
- Ternary diagram with confidence region for the matrix of coefficients of the SCLS or the TFLR model, [199](#)
- Ternary diagram with confidence region for the mean, [200](#)
- Ternary diagram with the coefficients of the simplicial-simplicial regression models, [201](#)
- ternary.coef (Ternary diagram with the coefficients of the simplicial-simplicial regression models), [201](#)
- ternary.coefcr (Ternary diagram with confidence region for the matrix of coefficients of the SCLS or the TFLR model), [199](#)
- ternary.mcr, [197](#), [198](#), [200](#)
- ternary.mcr (Ternary diagram with confidence region for the mean), [200](#)
- ternary.reg, [197](#), [201](#), [202](#)
- ternary.reg (Ternary diagram of regression models), [198](#)
- tflr, [43](#), [72](#), [157–161](#), [190](#), [200–202](#), [213](#), [227–229](#)
- tflr (The transformation-free linear regression (TFLR) for compositional responses and predictors), [230](#)
- tflr.betest, [158](#)
- tflr.betest (Permutation test for the matrix of coefficients in the TFLR model), [160](#)
- tflr.indeptest, [159](#), [161](#)
- tflr.indeptest (Permutation linear independence test in the TFLR model), [157](#)
- tflr2 (The TFLR model with multiple compositional predictors), [228](#)
- The additive log-ratio transformation and its inverse, [202](#)
- The alpha-distance, [203](#)
- The alpha-IT transformation, [205](#)
- The alpha-IT-distance, [206](#)
- The alpha-k-NN regression for compositional response data, [207](#)
- The alpha-k-NN regression with compositional predictor variables, [208](#)
- The alpha-kernel regression with compositional response data, [210](#)
- The alpha-SCLS model, [211](#)
- The alpha-TFLR model, [212](#)
- The alpha-transformation, [213](#)
- The Box-Cox transformation applied to ratios of components, [215](#)
- The ESOV-distance, [216](#)
- The folded power transformation, [217](#)
- The Frechet mean for compositional data, [218](#)
- The Helmert sub-matrix, [219](#)
- The k-nearest neighbours using the alpha-distance, [220](#)
- The k-NN algorithm for compositional data, [222](#)
- The multiplicative log-ratio transformation and its

- inverse, [224](#)
- The pivot coordinate transformation and its inverse, [225](#)
- The SCLS model, [226](#)
- The SCLS model with multiple compositional predictors, [227](#)
- The TFLR model with multiple compositional predictors, [228](#)
- The transformation-free linear regression (TFLR) for compositional responses and predictors, [230](#)
- Total variability, [231](#)
- totvar (Total variability), [231](#)
- Tuning of the alpha-generalised correlations between two compositional datasets, [232](#)
- Tuning of the bandwidth  $h$  of the kernel using the maximum likelihood cross validation, [233](#)
- Tuning of the divergence based regression for compositional data with compositional data in the covariates side using the alpha-transformation, [235](#)
- Tuning of the k-NN algorithm for compositional data, [236](#)
- Tuning of the projection pursuit regression for compositional data, [239](#)
- Tuning of the projection pursuit regression with compositional predictor variables, [240](#)
- Tuning of the projection pursuit regression with compositional predictor variables using the alpha-transformation, [241](#)
- Tuning the number of PCs in the PCR with compositional data using the alpha-transformation, [243](#)
- Tuning the parameters of the regularised discriminant analysis, [245](#)
- Tuning the principal components with GLMs, [246](#)
- Tuning the value of alpha in the alpha-regression, [248](#)
- tv.compreg (Divergence based regression for compositional data), [69](#)
- Two-sample test of high-dimensional means for compositional data, [250](#)
- ulc.glm, [12](#), [115–117](#), [256](#)
- ulc.glm (Unconstrained GLMs with compositional predictor variables), [251](#)
- ulc.glm2, [116](#), [117](#), [252](#), [258](#)
- ulc.glm2 (Unconstrained logistic or Poisson regression with multiple compositional predictors), [255](#)
- ulc.reg, [13](#), [121–123](#), [255](#)
- ulc.reg (Unconstrained linear regression with compositional predictor variables), [252](#)
- ulc.reg2, [123](#), [253](#)
- ulc.reg2 (Unconstrained linear regression with multiple compositional predictors), [254](#)
- ulc.rq, [118–120](#), [259](#)
- ulc.rq (Unconstrained quantile regression with compositional predictor variables), [257](#)
- ulc.rq2, [120](#)
- ulc.rq2 (Unconstrained quantile regression with multiple compositional predictors), [258](#)
- Unconstrained GLMs with compositional predictor variables, [251](#)
- Unconstrained linear regression with compositional predictor variables, [252](#)
- Unconstrained linear regression with multiple compositional predictors, [254](#)
- Unconstrained logistic or Poisson regression with multiple compositional predictors, [255](#)
- Unconstrained quantile regression with compositional predictor variables, [257](#)
- Unconstrained quantile regression with multiple compositional predictors, [258](#)

Unit-Weibull regression models for proportions, [260](#)  
unitweib.reg (Unit-Weibull regression models for proportions), [260](#)  
unitweibull.est (MLE of distributions defined in the  $(0, 1)$  interval), [131](#)

zad.est, [262](#)  
zad.est (MLE of the zero adjusted Dirichlet distribution), [137](#)  
zadr, [8](#), [64](#), [137](#)  
zadr (Zero adjusted Dirichlet regression), [261](#)  
zadr2 (Zero adjusted Dirichlet regression), [261](#)  
Zero adjusted Dirichlet regression, [261](#)  
zeroreplace, [137](#)  
zeroreplace (Non-parametric zero replacement strategies), [155](#)  
zilogitnorm.est, [137](#)  
zilogitnorm.est (MLE of distributions defined in the  $(0, 1)$  interval), [131](#)